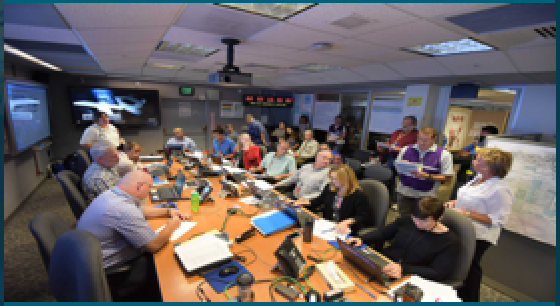
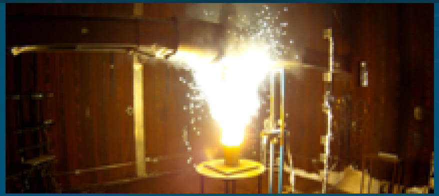
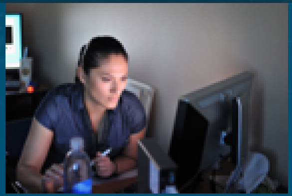
SAND2023-03457T

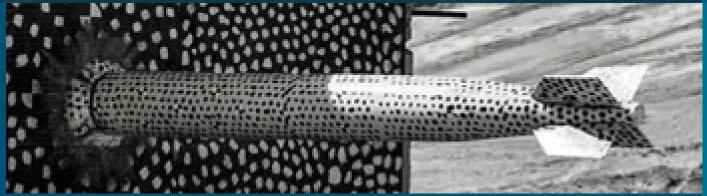
Sandia National Laboratories

Simulating LC Circuits in Cylindrical Photoemission Driven Cavities Using Coupled Monte Carlo and Particle-in-Cell Codes









PRESENTED BY

Ravi Shastri[1,2]

[1] Sandia National Laboratories: Radiation Effects Experimentation

Motivation

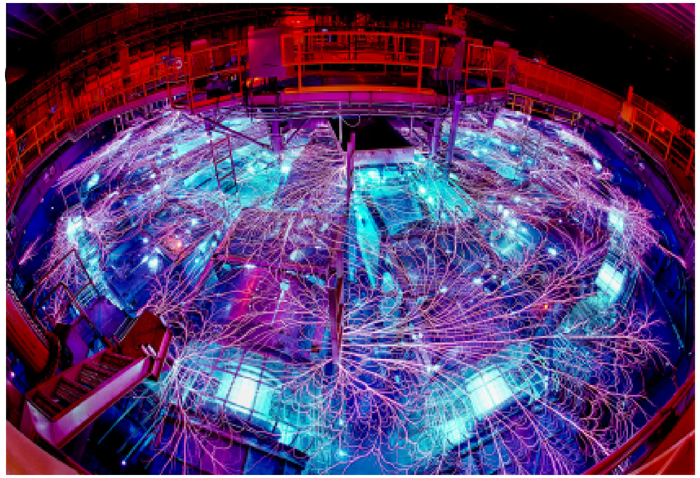
- Use coupled Monte-Carlo and Particle-in-Cell codes to simulate the physics of a photoemission driven anode/cathode gap
- Model current measured by a B-Dot diagnostic when a fill gas is added to the anode/cathode gap, and when accounting for space-charge limited emission
- Model the simulation in two parts: the gas filled cavity and a transmission line
- Demonstrate that coupling a transmission line to an anode/cathode gap produces similar physics
- Improve computational efficiency by using this configuration
  - Show that a simplified model with a transmission line produces similar output currents to a full simulation
- Compare transmission line current outputs to simulated data for 1 mm and 10mm cavities
  - Use a stainless-steel and silver spectra from experiment
- Explore implications of modeling a transmission line for other diagnostics

Outline

- Introduction
- Background Physics
- Methods
- Results
- Discussion
- Conclusion and References
- Acknowledgements and Questions

Introduction

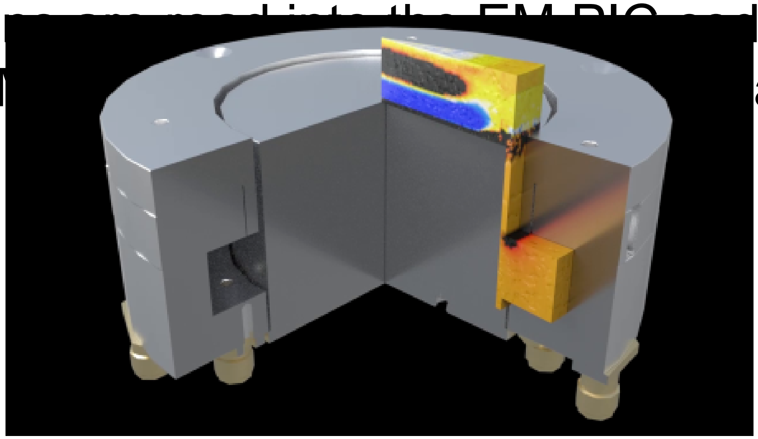
- Pulsed Power Shots on the Z Machine
  - Pulsed power accelerator that can reach 80TW of power
- Simulate Radiation Transport
  - Photons and photoelectrons
- Purpose
  - Understand how exposure to radiation affects electrical systems
  - Ensure functionality of electrical equipment in hostile environments
- Objective: Understand the physics in a cylindrical photoemission driven cavity, and use high performance computing to simulate current and voltage output from experiments driven using the Z machine.
- Relevant Physics
  - Plasma Physics: Space-charge limited emission **(S**
  - LC Circuits
  - Material emission spectra
  - Electromagnetic **(EM)** Simulation



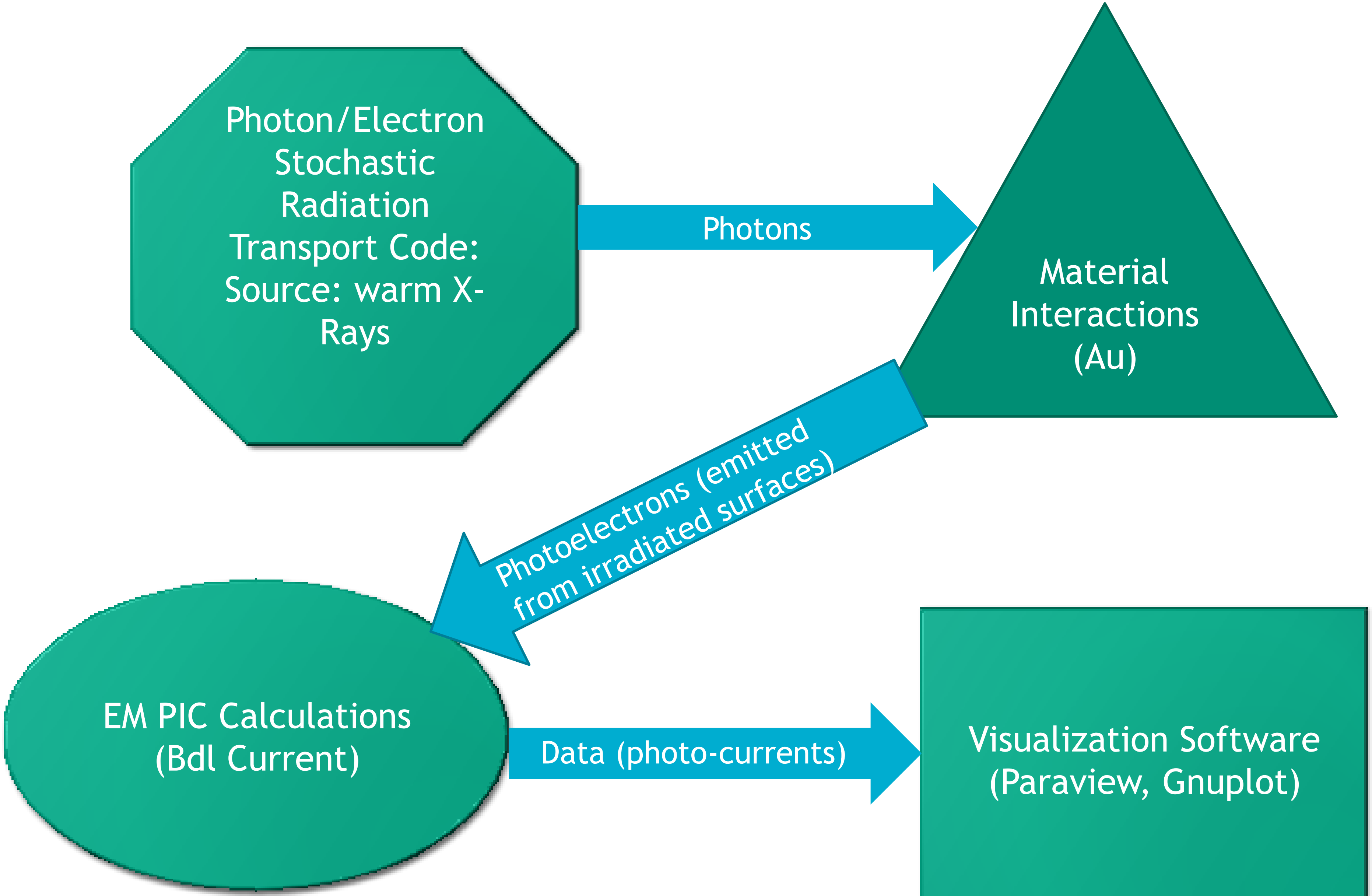
Z-Machine

Introduction

- Experimentally measured x-rays are computationally transported into an anode/cathode **(A/K)** gap
  - Monte Carlo (MC) photon/electron transport code
- This creates photoelectrons, which are emitted from the surfaces into a cavity
  - The top surface is Al with a carbon coating to suppress photoelectron emission
  - The bottom surface is the irradiated material; photoelectron spectrum changes with material
    - Possible materials include Au, Ni, Ti, Mo, Y, but this presentation will focus on Au's photoelectron emission
- Not a single frequency x-ray source
  - Photo-electron spectrum ranging from 1 – 32 keV
  - Emitted electro
- After running the E antities are visualized using ParaView



Cavity Geometry


Photon/Electron Stochastic Radiation Transport Code: Source: warm X-Rays
Photons
Material Interactions (Au)
Photoelectrons (emitted from irradiated surfaces)
EM PIC Calculations (Bdl Current)
Data (photo-currents)
Visualization Software (Paraview, Gnuplot)

Diagnostic - BDot

- The current measurement diagnostic used in our experiment is called a **B-Dot** [1]
  - B-Dot ($\dot{B}$) comes from $\frac{dB}{dt}$, or the changing magnetic field induced by current flowing in the circuit [2]
  - The x-ray pulse creates photoelectrons that are excited, emitted, and transported across the gap, creating a current, and inducing a magnetic field in the sensor cavity, producing a voltage in the sensor circuit [3]
  - Bdl current: $\mu_0 I = \int \vec{B} \cdot d\vec{l}$
- 1 mm and 10 mm cavities
- Stainless-Steel and Silver x-ray spectra

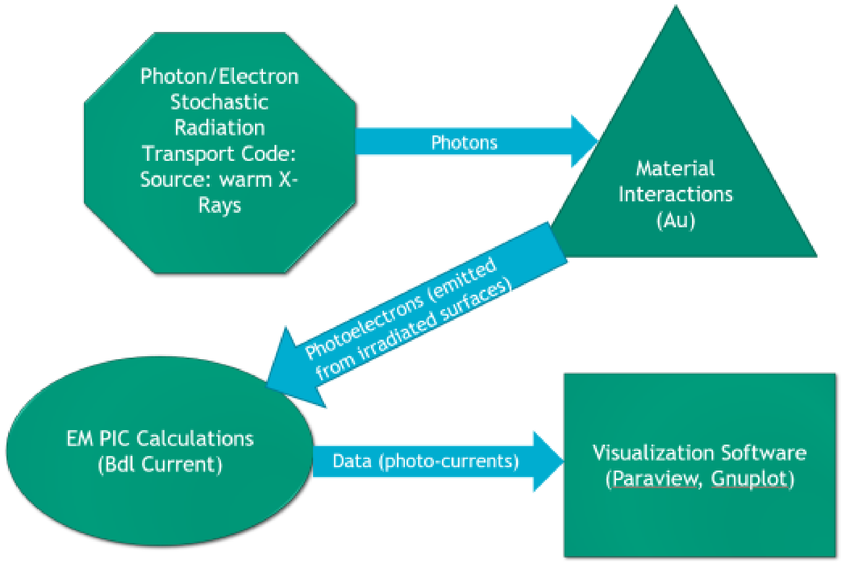
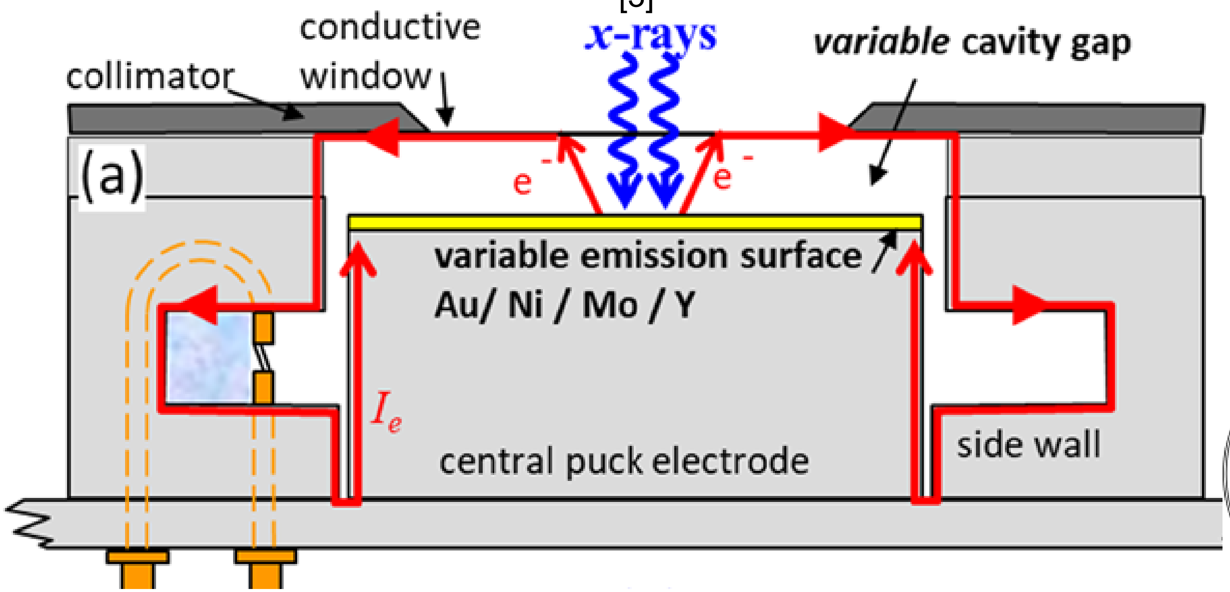


Figure 1: B-Dot schematic sketch. Not drawn to scale [3]



Plasma Physics and LC Circuit Modeling

- Current method: model entire system
  - Gas Filled Cavity, B-Dot sensor region, and the stem connecting the 2 blocks
- Tim Flanagan paper: LC circuit model for cylindrical cavity with B-Dot diagnostic
  - Models 1 mm vacuum B-Dots and LB-Dots
- Adding Plasma Physics from gas filled cavity
- Model gap as photoelectron emission driven cavity, model diagnostic and stem as an **LC circuit**
- **Show that output is the same for a full simulation of the geometry and a separation of the cavity**

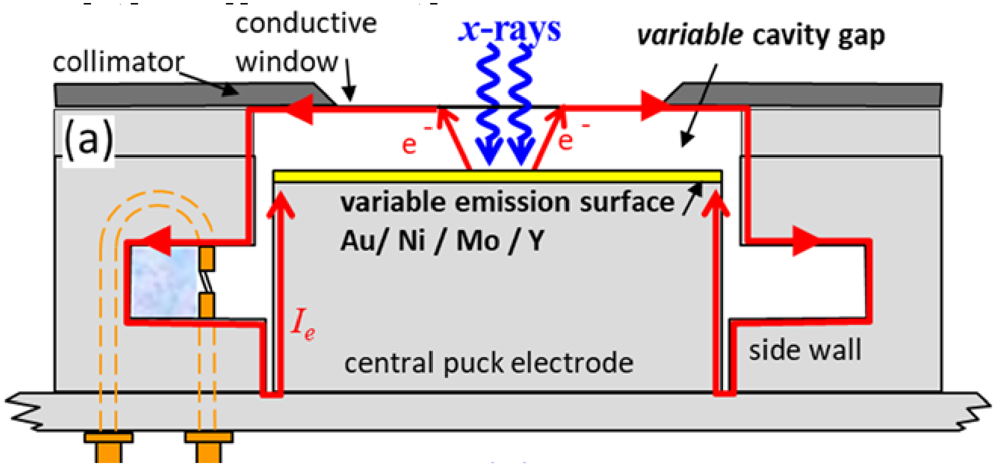
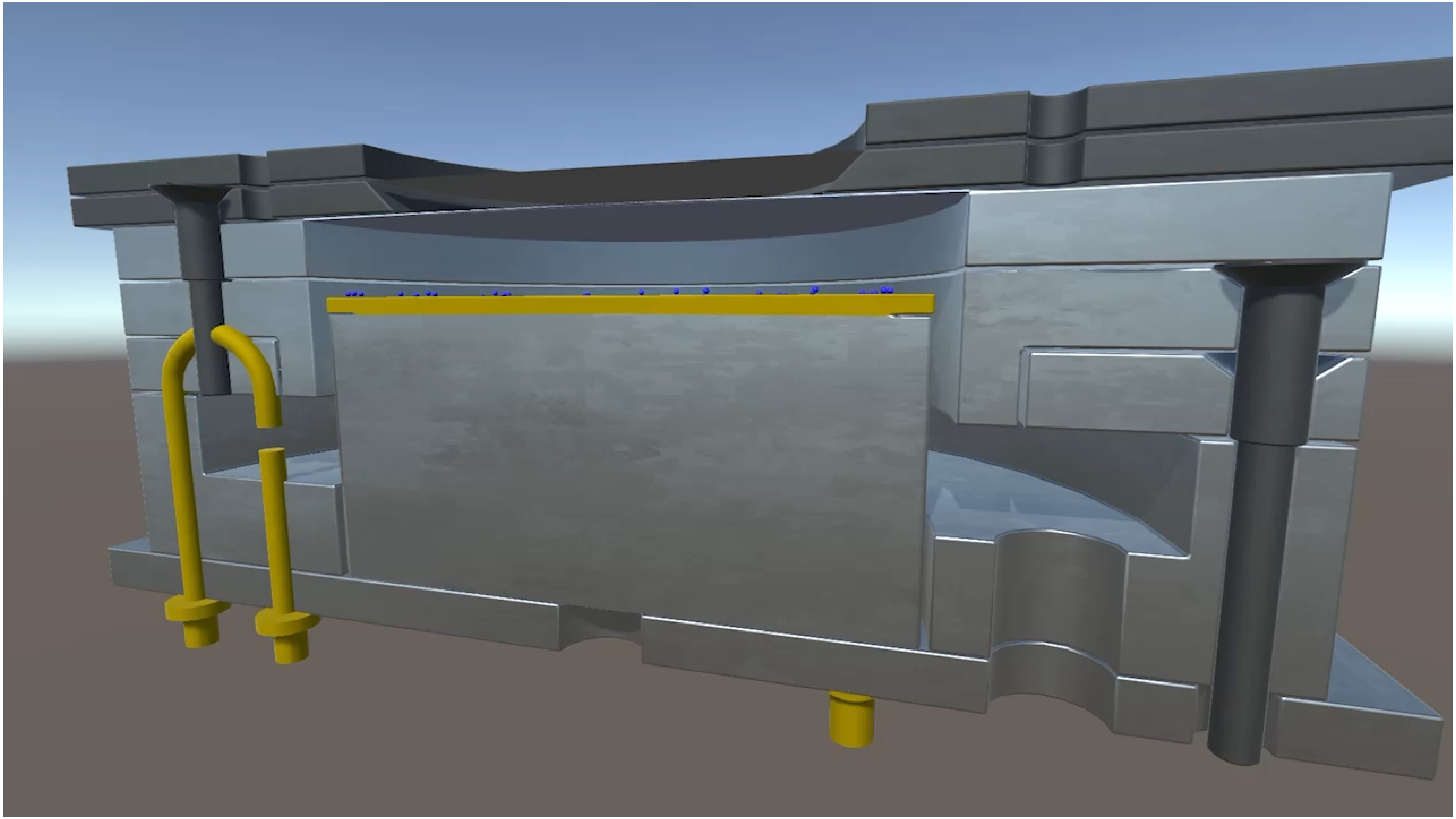
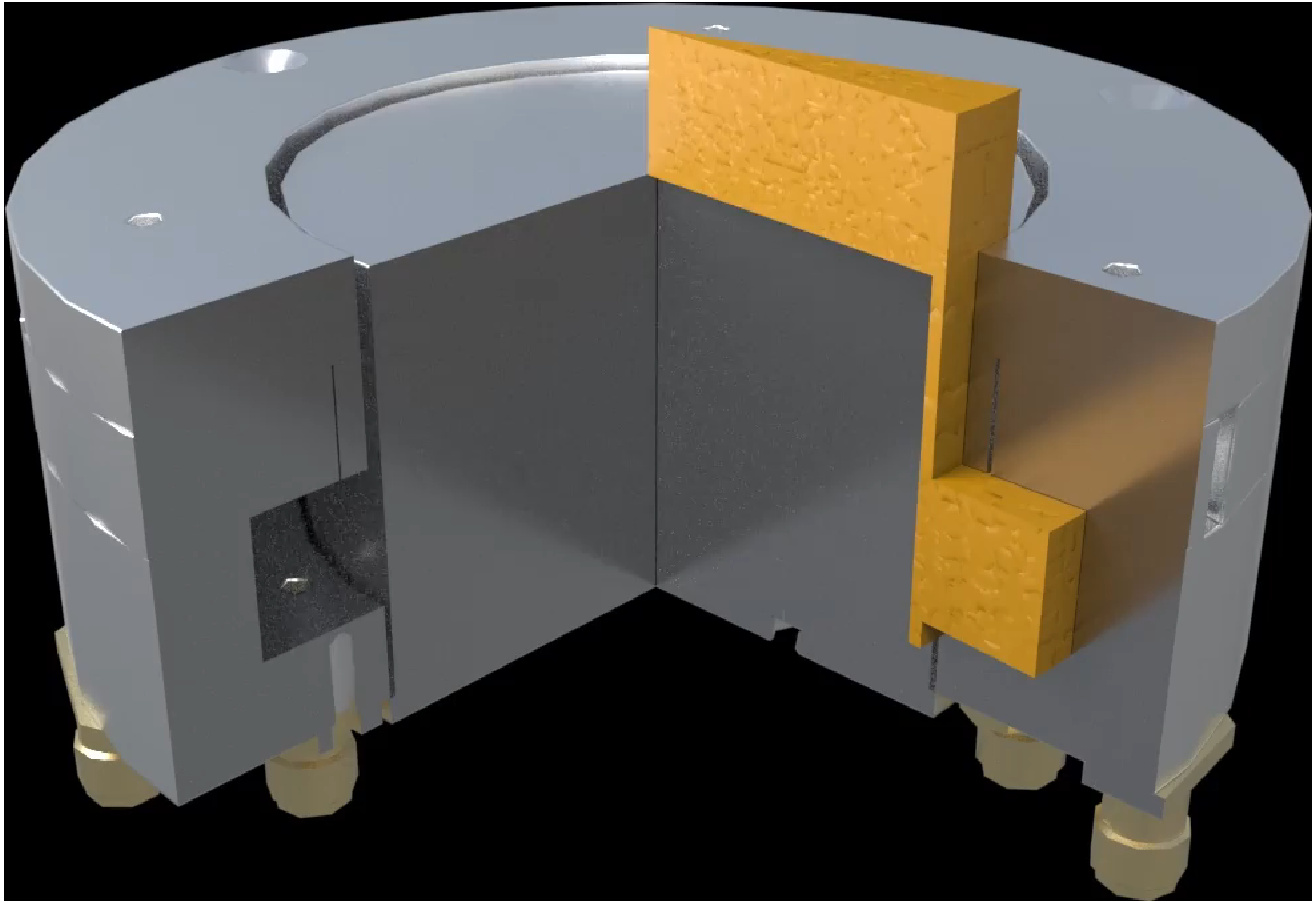


Figure 1: B-Dot schematic sketch. Not drawn to scale [3]

Visualization



Visualization



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Child-Langmuir Law: Space-Charge Limited Emission

- There is a fundamental limit on the current density transmitted across a cavity or AK gap, which is the **space-charge limit (SCL)** between two electrodes [4]
  - This effect comes from electron self-interaction and Coulomb's law
  - Electrons must have enough kinetic energy after photoelectric emission to overcome the coulomb barrier and traverse the gap
  - The electric field dictates the direction of the electrons
- **The SCL current represents the maximum current that can be transmitted across an AK gap**
  - It corresponds to a surface electric field of zero, where the electron charge density has shielded the electric field at the cathode so that electrons emitted with a zero velocity will no longer be accelerated into the gap
- The 1-D Child-Langmuir limited current density is given by equation 1 [6]
  - Note the $V^{3/2}/d^2$ dependence

$$J_{CL} = \frac{4\epsilon_0}{9}\sqrt{\frac{2e}{m}}\frac{V^{3/2}}{d^2}. \qquad 1$$

LC Circuit Derivation with Initial Charge Q_0

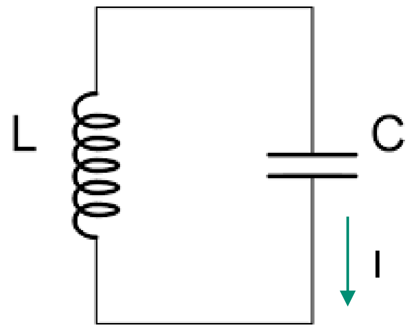


Figure 2: LC circuit sketch

Starting with Kirchoff's Law:

$$\sum V = 0$$

Where V is voltage across each element. We know that $V_0 = \varepsilon$, VC = qC, and $V_L = L\frac{dI}{dt}$, where C is capacitance, q is charge, L is inductance, and I is current. The voltage for each term is

$$V_0 - V_c - V_L = 0, \text{ or } V_0 = V_c + V_L, \text{ and } \varepsilon = qC + L\frac{dI}{dt}$$

Since this circuit is not driven, $\varepsilon = 0$. $I(t) = \frac{dq}{dt}$, therefore

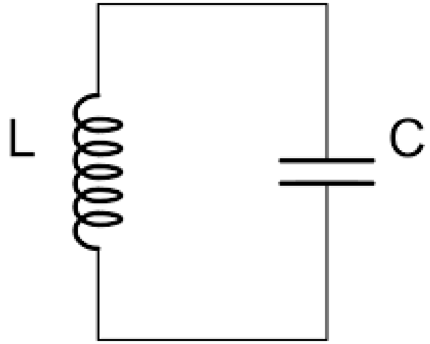
$$\left(\frac{d^2}{dt^2} + \frac{1}{LC}\right)q = 0$$

This is a simple 2nd order differential equation. Set $\frac{1}{LC} = \omega^2$. Solving for q(t), we have

$$q(t) = A\cos(\omega t) + B\sin(\omega t)$$

where ω is the resonant frequency [5]

LC Circuit Derivation with Initial Charge Q_0



The current is the time derivative of charge, so

$$I(t) = -A\,\omega\sin(\omega t) + B\,\omega\cos(\omega t)$$

$$q(t=0) = q_0$$

$$I(t=0) = 0$$

$$q(t) = A = q_0$$

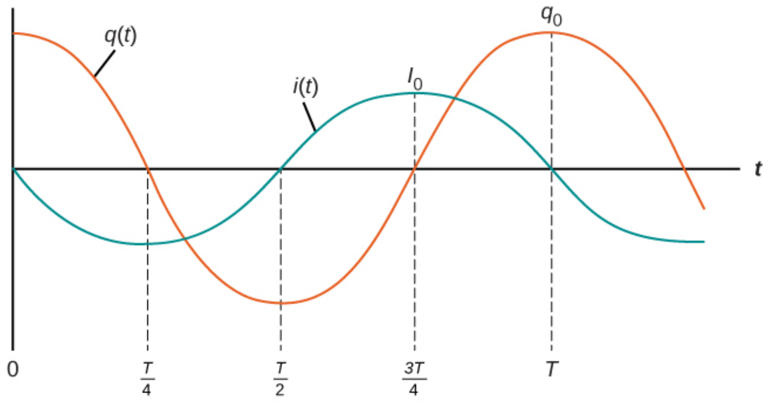
$$I = B\omega = 0, \omega \neq 0, \text{therefore } B = 0$$

Subbing in for ω,

$$q(t) = q_0 \cos\frac{t}{\sqrt{LC}} \qquad 2$$

$$I(t) = \frac{-q_0}{\sqrt{LC}}\sin\left(\frac{t}{\sqrt{LC}}\right) \qquad 3$$

Figure 3: LC circuit charge vs time (orange) and current (blue) vs. time



Q(t) and I(t) for Damped Circuits

- $\varepsilon = qC + L\frac{\mathrm{d}I}{\mathrm{d}t} + \mathrm{IR}$
- Q(t) and I(t) in the capacitor for an RLC Circuit
- Dampened RCL Circuit Critically Damped RLC Circuit($\beta = \omega_0$)

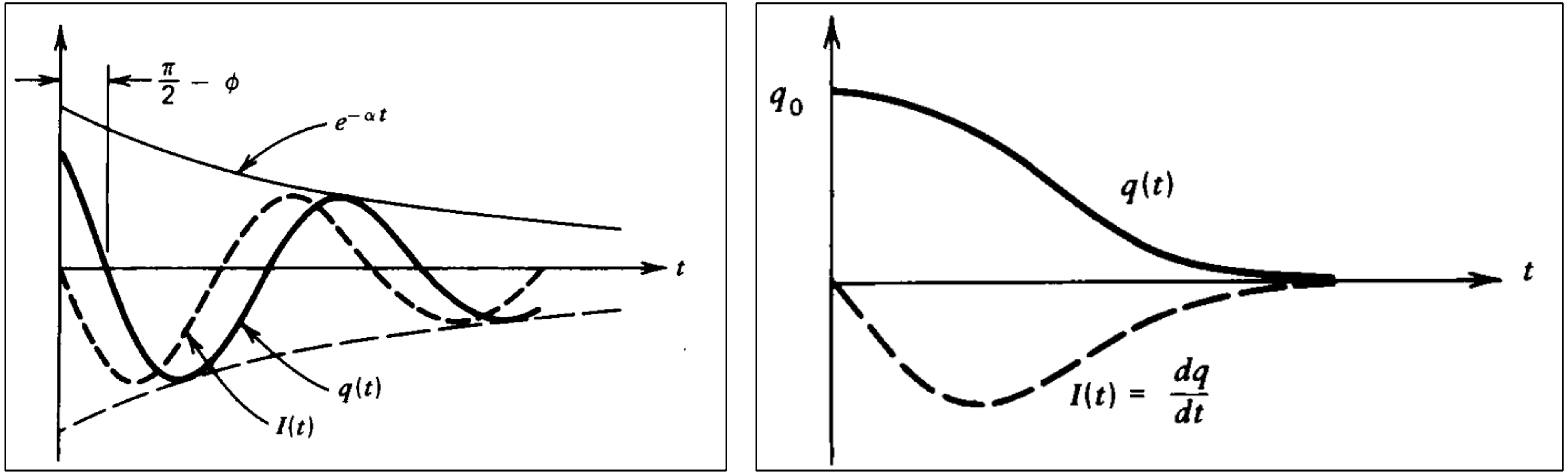


Figure 4: q(t) and I(t) for damped circuit. These diagrams are similar to modeling SCL emission in the transmission line simulations [6]

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Cavity Geometry

- Cylindrical end irradiated cavity
  - The gap size of the cavity is **10mm**
  - We will see 1 mm gap sizes as well
- The top surface is the **anode**
  - Aluminum, with a thin carbon layer
- The bottom surface is the **cathode**
  - Gold, where most of our photoelectron emission comes from
  - The photoelectron spectrum mainly consists of electrons moving from cathode to anode, although there is a small contribution from anode emission
- This snapshot is for electron emission with low pressure N_2 fill gas at 11.4ns from ParaView

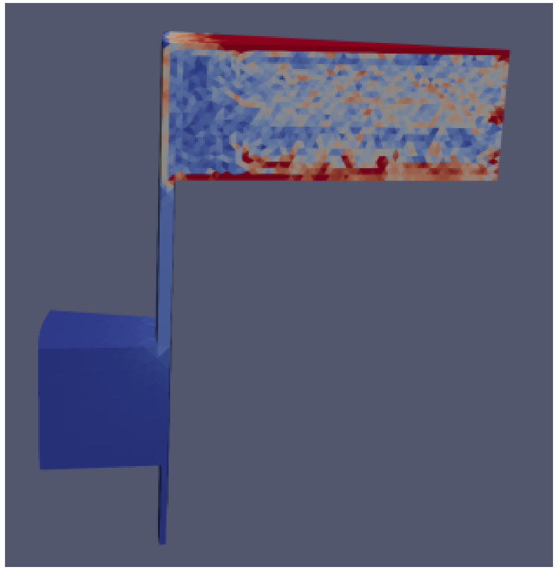


Figure 5a: profile view of the cavity geometry. The cavity is the rectangular wedge, and the B-Dot diagnostic is the block on the bottom

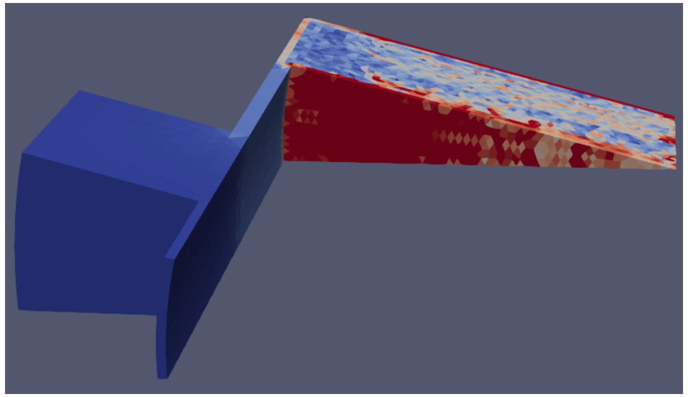
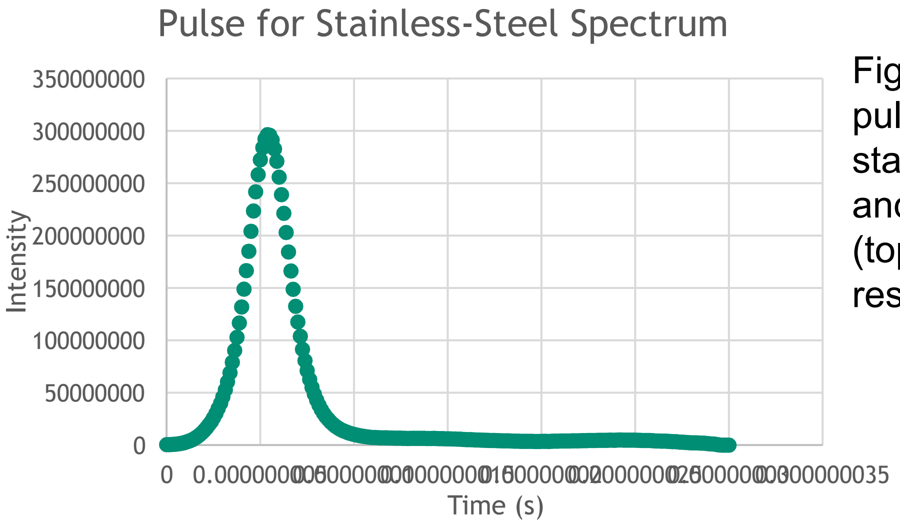


Figure 5b: bottom surface view of the cavity geometry

Methods

- Stainless-Steel Time pulse: 3ns FWHM pulse from Z
- Silver Time pulse: 1.5ns FWHM pulse from NIF
- Surface 1 filters: Kapton, C, Li
  - Filters out low energy photons (below 1keV)
  - 50cm from cathode
- Au is a strong emitter and can create rather large currents in the cavity compared to Ni, Ti, and other D block metals.



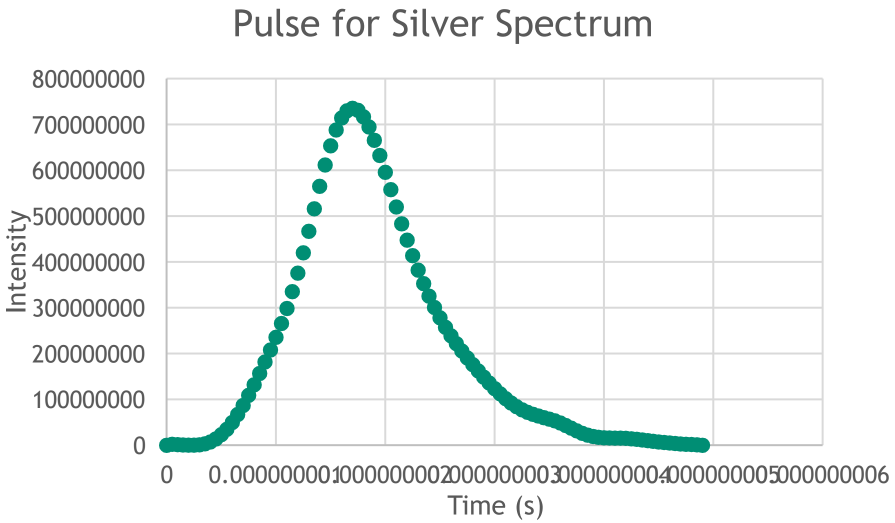


Figure 6: Time pulse used in stainless-steel and silver spectra (top and bottom) respectively

Monte Carlo Photon/Electron Code: Photoemission Driven Cavities Input Spectra- Stainless-Steel

- Input spectrum: Z pinch stainless-steel wire array
  - 50cm from the Au surface
  - 20keV max energy
- The cathode's peak emission is more than an order of magnitude larger than the anode's peak emission
  - Therefore, the **cathode is the predominant emitter**

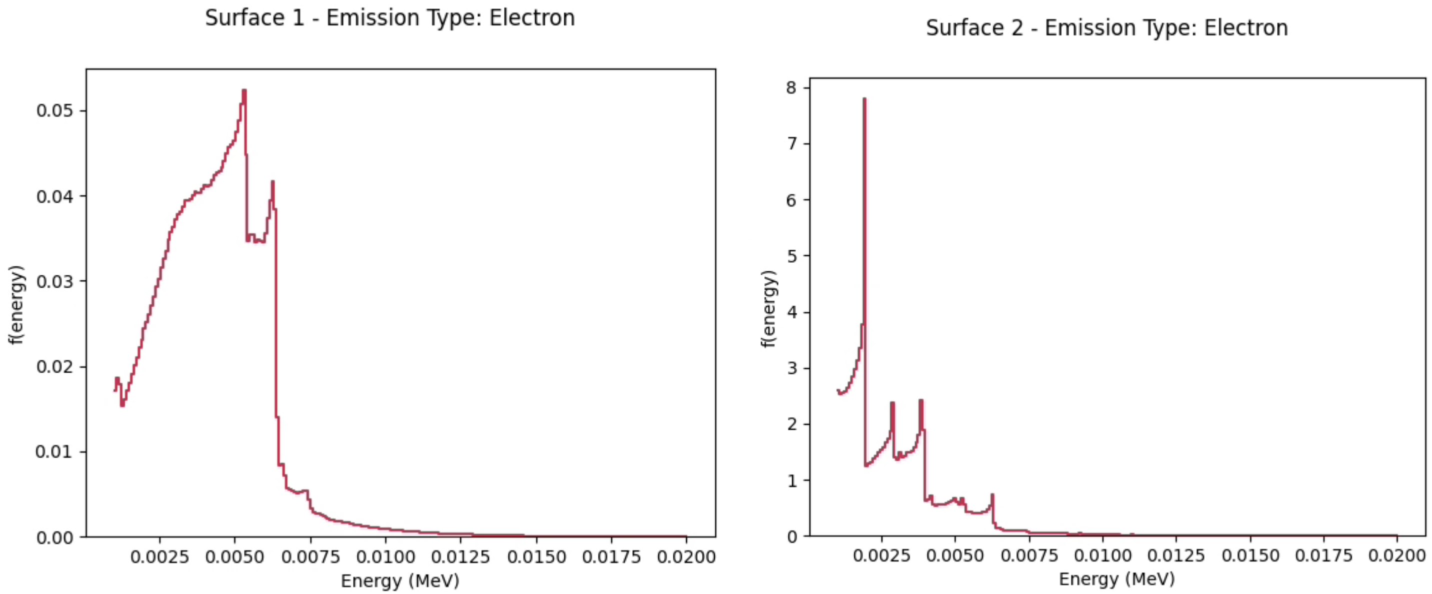
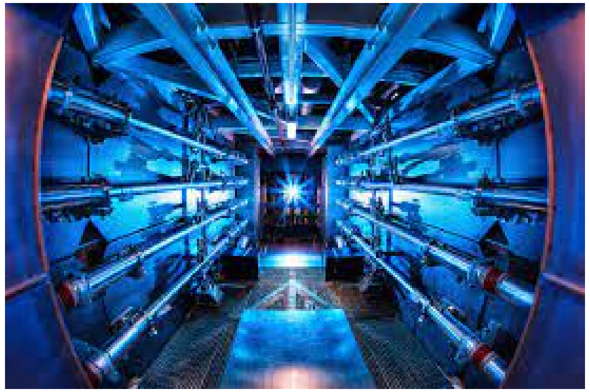
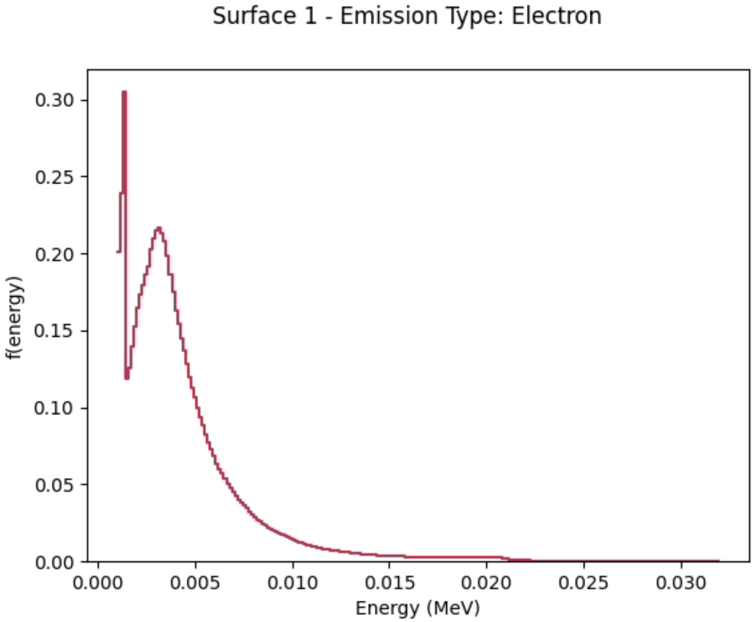


Figure 7: Photoelectron emission spectra for AK gap from the top (anode) (left) and bottom (cathode) (right) surfaces, stainless-steel spe

Monte Carlo Photon/Electron Code: Photoemission Driven Cavities Input Spectra- Silver

- Input spectrum: Silver spectrum from NIF
  - 31.7cm from the Au surface
  - 32keV max energy emission
- The cathode’s peak emission is more than an order of magnitude larger than the anode’s peak emission
  - Therefore, the **cathode is the predominant emitter**





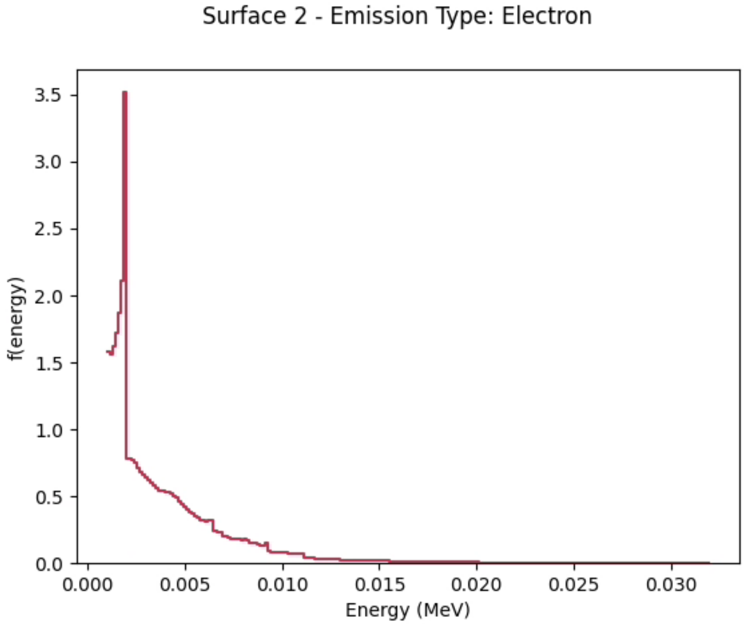


Figure 8: Photoelectron emission spectra for AK gap from the top (anode) (left) and bottom (cathode) (right) surfaces, silver spe

EM PIC Input Requirements

- The photoelectron spectrum is sent to the EM PIC code
- This is where we can change pressure, fill gas, meshing, and toggle SCL on/off
- The main measured output is Bdl current, or the current measured by the B-Dot
- More information about the EM PIC code can be found in reference [7]

Transmission Line Modeling

- The simulation provided us with good results that are similar to experiment
- However, these simulations require many computation hours and rather large mesh sizes
- This is where we can split the bodies of the geometry and model the plasma A/K gap physics fully, and model the EM circuit as a transmission line
- Simplifies the geometry, allows for finer meshes, reduces computation hours, and can be applied to any EM diagnostic easily
- The solution changes slightly if the AK gap is driven (X-ray diode)

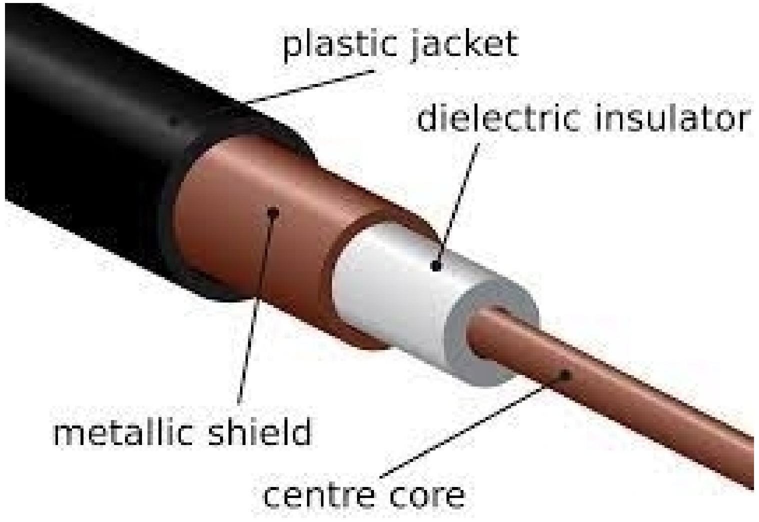
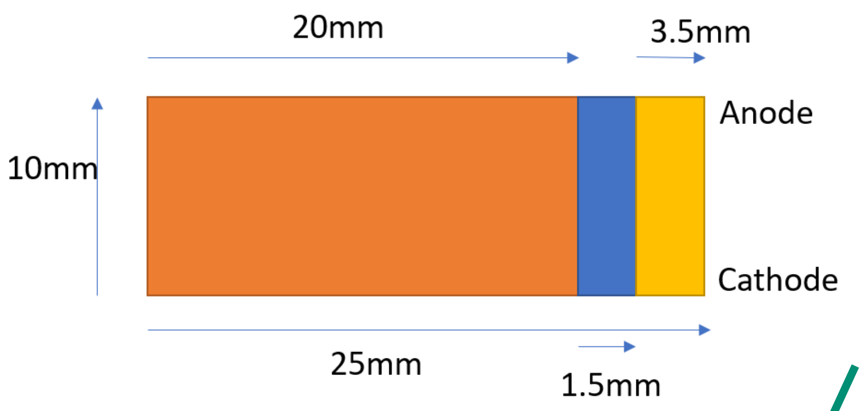


Figure 9: Sketch of coaxial cable transmission line

Radial TL EM PIC Requirements

- A more efficient way to model this system is to divide it into two parts
  - **The gas filled cavity with an AK gap, and a transmission line (TL)**
- Consider the profile of the cavity wedge
- The orange region is the emission region
  - The anode and cathode extend the full 25 mm
- The right edge of the yellow region (the outer radius) is the transmission line
- The blue region is the penumbral region
  - It could see x-rays if they came in at an angle. The shadow of the photon flux can enter this region, but there should be no photon flux by the yellow region and TL
- The highlighted orange lines are the nodes created to model the transmission line.
- Only tetrahedral (tet) meshes are supported

Figure 10: Radial TL cavity profile regions



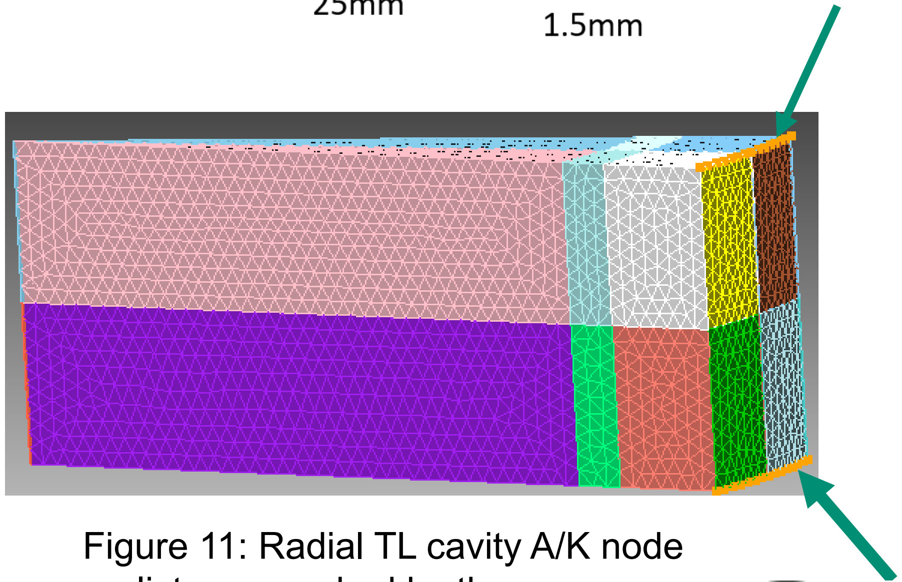
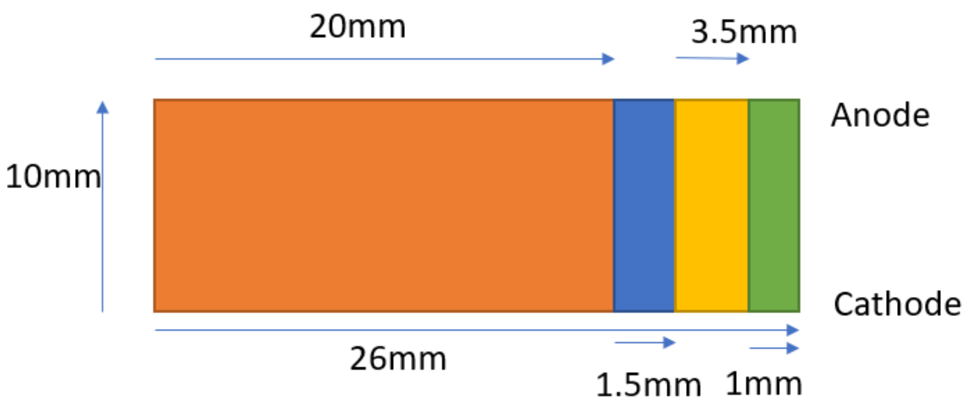


Figure 11: Radial TL cavity A/K node lists, as marked by the arrows

Axial TL EM PIC Requirements

- Consider the profile of the cavity wedge
- The orange region is the emission region
  - The anode and cathode extend the full 25 mm
- The right edge of the yellow region (the outer radius) is tl transmission line
- The blue region is the penumbral region
  - It could see x-rays if they came in at an angle. The shadow of the photon flux can enter this region, but there should be no photon flux by the yellow region and TL
- The green region is the stem
  - The bottom of the stem connects to the B-Dot. We can model our LC circuit and Transmission line here
- The highlighted orange lines are the nodes created to model the transmission line.
- Only tet-meshes are supported

Figure 12: Axial TL cavity profile regions



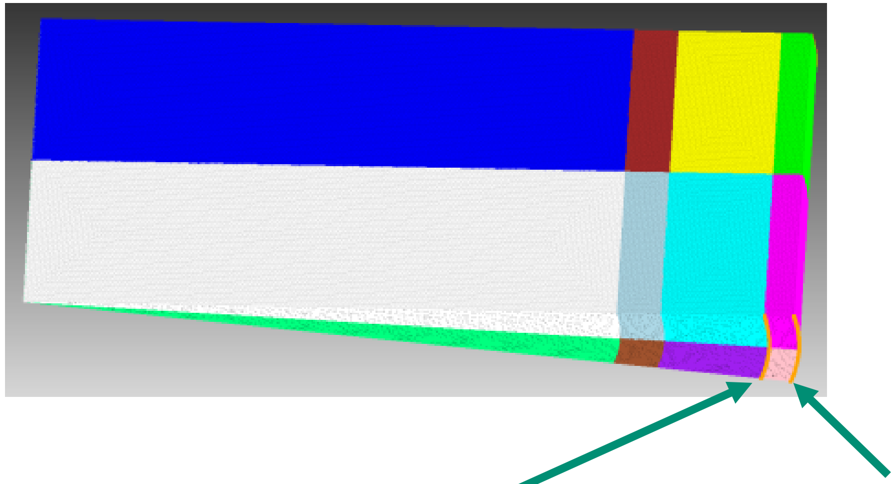


Figure 13: Axial TL cavity A/K node lists

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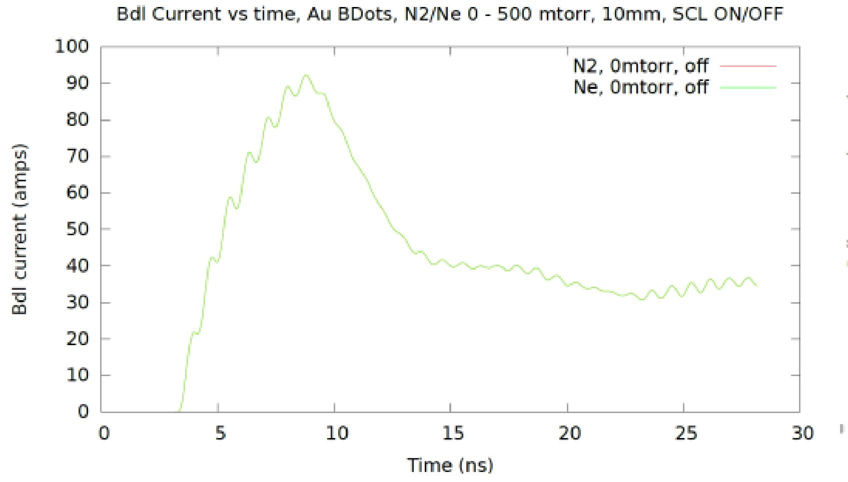
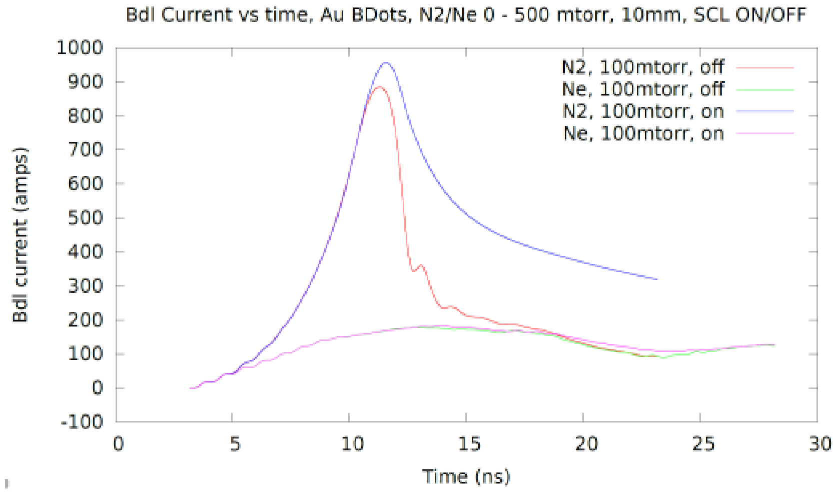
Low Pressure N_2 and Ne

- Ne and N_2 at vacuum are the same
- At 200 mTorr, N_2 has a higher peak current than Ne, and peaks earlier
- SCL: the EM PIC code drives the maximum current through the circuit when toggled "on", and ignores these effects when toggled "off" [3]
- Since N_2 is diatomic, it is easier to ionize at lower pressures than Ne
  - This is why we see higher peak currents at low pressures.





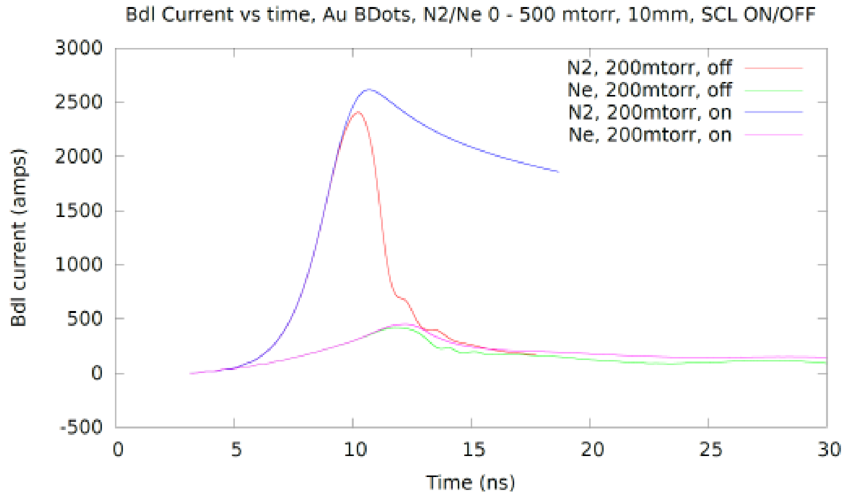


Figure 14: Bdl current vs time for Ne and N_2 B-Dot simulations below 200 mTorr. Au is the cathode emitter, and the gap is 10mm. SCL emission is toggled on/off

Circuit Modeling: Radial

- The way we bring in the Transmission Line matters
- Radial TL
  - Equidistant from the center of the cavity
  - TL modeled on between the AK gap
- Lumped Element LC circuit modeling

```
Transmission line on sideset
  C_l = 5.79496e-12
  L_l = 1.92003e-06

***************************************************
Circuit Network: TL z_0
Network Junctions:
  Junction_0 EM Coupling Junction
    Attached to (Cable , Conductor, Side):
        (0,0,right)
  Junction_1 External Resistor
    Attached to (Cable , Conductor, Side):
        (0,0,left) Resitance 575.611 (Ohms)
Network Cables:
  0: TL z TEM Mode
     Number of Conudctors: 1
***************************************************
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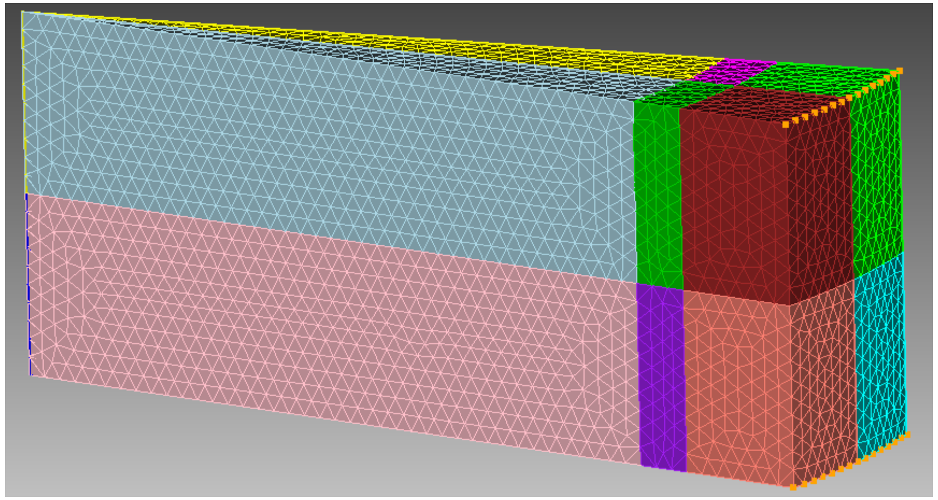


Figure 15: 10mm B-Dot with Transmission line brought in radially, with nodes on the A/K edges

Problems with Radial TL

- The code calculates the L and C from the sideset
- $R_{Sideset} = \sqrt{L/C}$
- Changing relative permittivity and permeability does not change the balance of the circuit in the presence of a plasma
- The Bdl current output is the same for every pressure
  - This is not physical, and does not match experiment or simulation
- The current also peaks too early, we expect to see a peak between 10 and 15 ns
- Circuit block available in the appendix

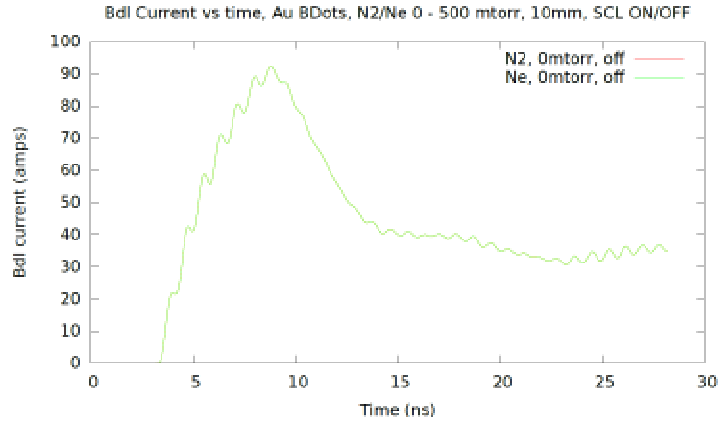


Figure 16: Radial transmission line modeled on outer sideset of meshed cavity geometry

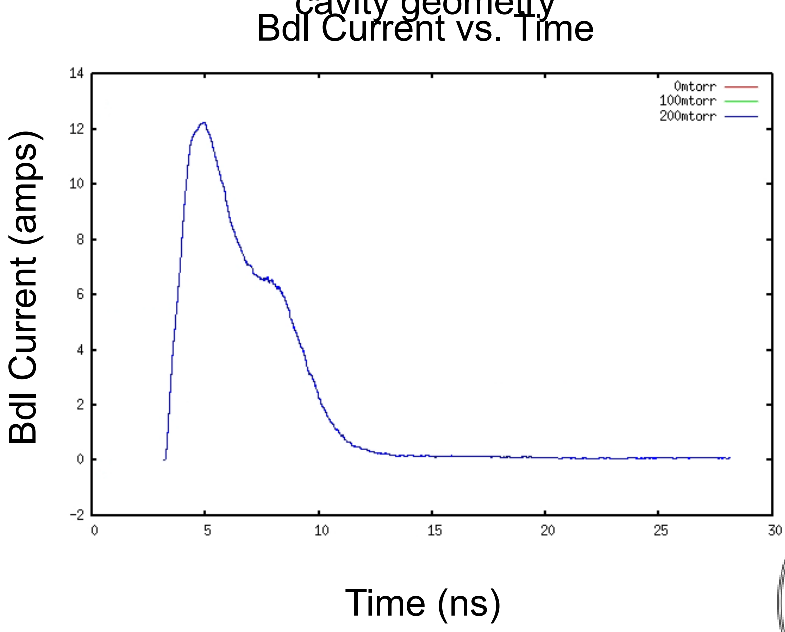


Figure 17: Bdl current vs time for a 10mm Au B-Dot between 0 and 200 mTorr, with balance modeled as radial transmission line

Circuit Modeling: Axial

- Transmission line modeled at the same height (z) on the cathode
- No longer lumped LC circuit
- L and C are calculated for a Coaxial Cable in equations 4 and 5, where ‘b’ is outer radius and ‘a’ is inner radius [3]
- Finer mesh is required
- The part of the stem that connects to the cavity is now modeled and meshed.

$$C = \frac{2\pi\varepsilon_0\varepsilon_r}{\ln\left(\frac{b}{a}\right)} \quad F/m \qquad (4)$$

$$L = \frac{\mu_0\mu_r}{2\pi}\ln\left(\frac{b}{a}\right) \quad H/m \qquad (5)$$

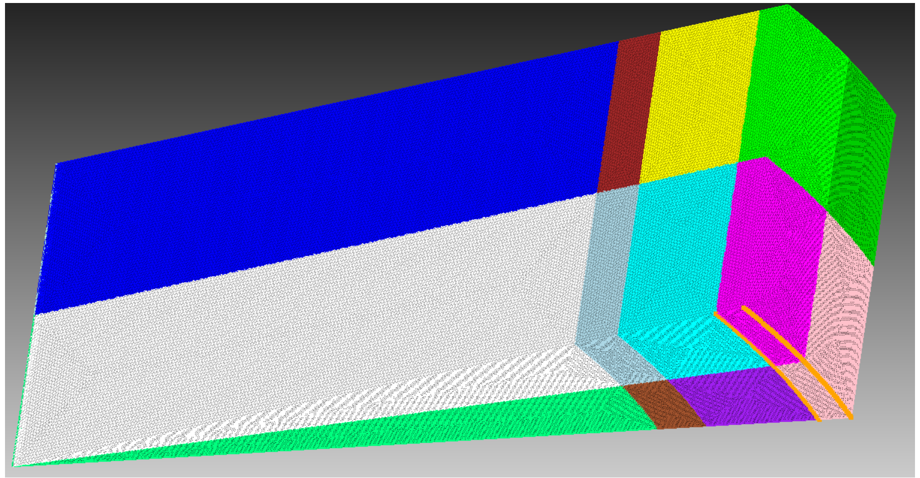
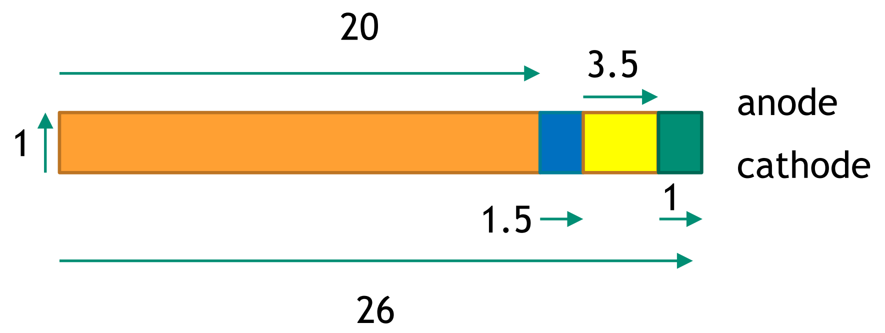


Figure 18: 10mm B-Dot with Transmission line brought in axially, with nodes connecting to the stem

Circuit Modeling: Axial 1 mmV

- All dimensions are in mm
- 1 mm cavity height
- The orange region is the emission region
  - The anode and cathode extend the full 25 mm
- The right edge of the yellow region (the outer radius) is the transmission line
- The blue region is the penumbral region
- The green region is the stem
  - The bottom of the stem connects to the B-Dot. We can model our LC circuit and Transmission line here

Figure 19: Axial TL cavity profile regions, 1 mm



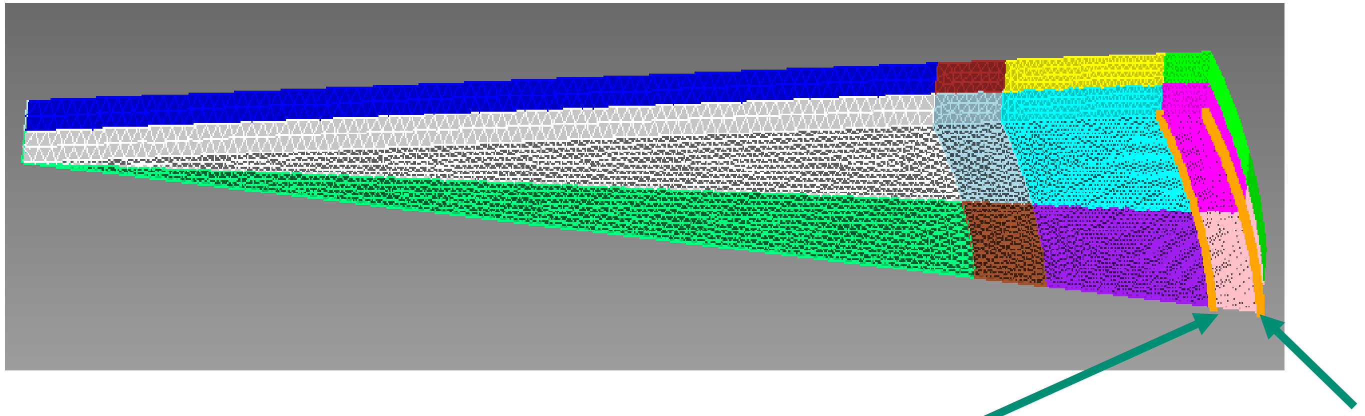


Figure 20: Axial TL cavity A/K node lists

1 mm B-Dot Full Simulation Results

- 1 mm cavity, Ne fill gas, low pressure
- Stainless-Steel input spectrum
- Basis of comparison for transmission line simulations

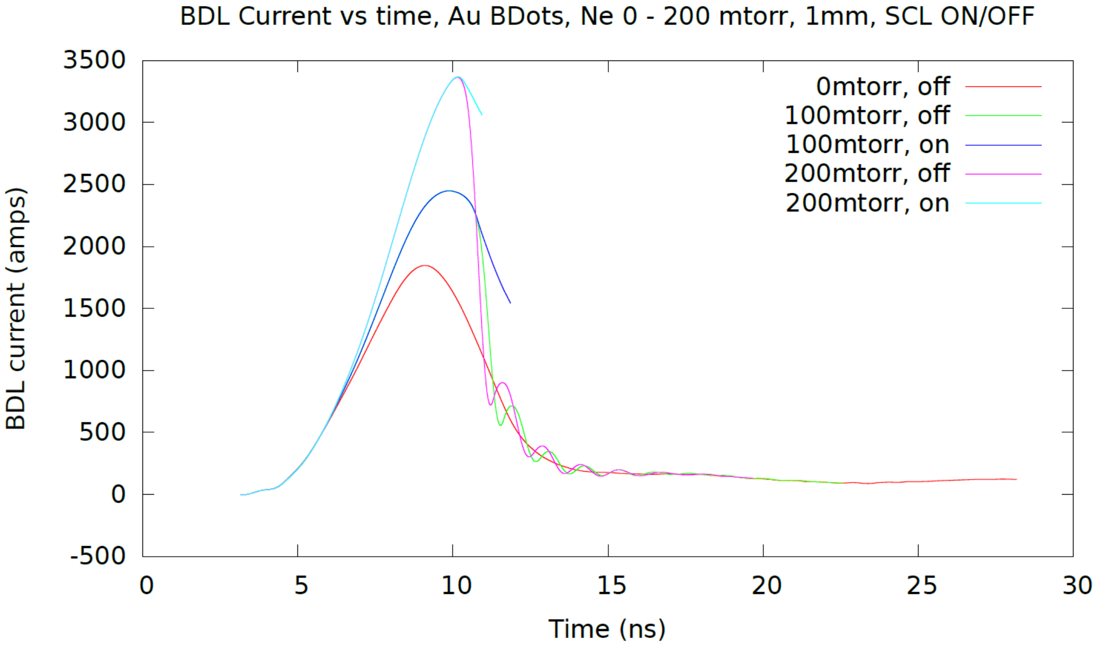


Figure 21: Bdl current vs time for a 1 mm Au B-Dot system between 0 and 200 mTorr Ne fill gas full simulation results, stainless-steel input spectrum

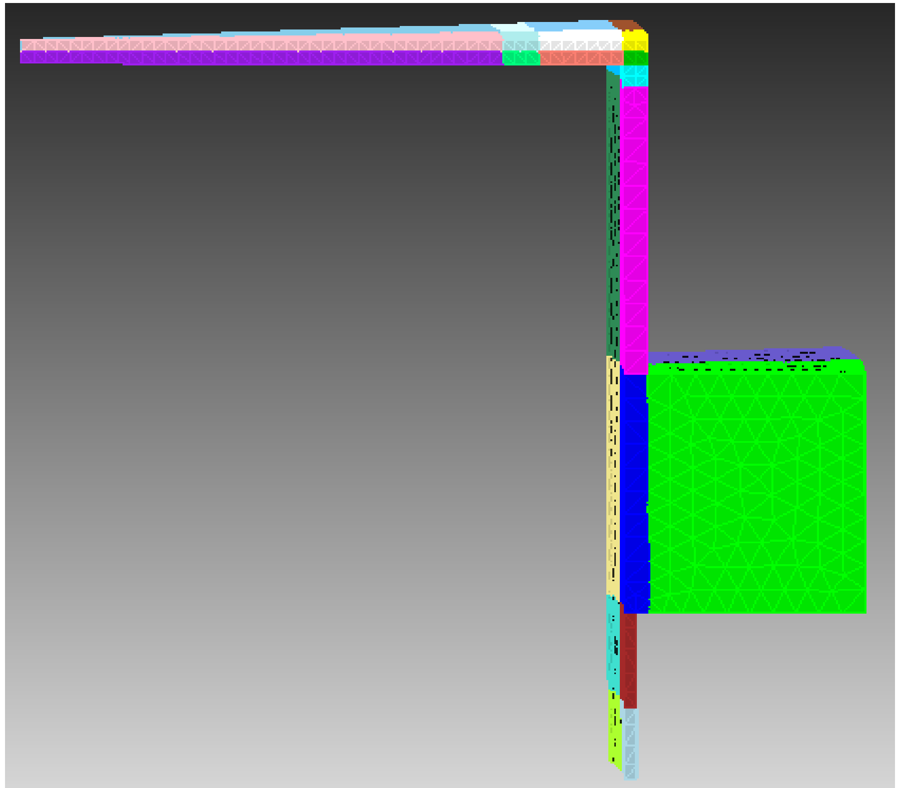


Figure 22: 1 mmN B-Dot full geometry.

1 mm B-Dot Full Simulation Results: N vs V

- N: sensor cavity radius = 35 mm
- V: sensor cavity radius = 30.5 mm
- This does not affect our geometry in the transmission line simulation, but it does change the values for L and C
  - Are these changes in LC significant?
  - In short, no
  - Slightly different rise time and peak current, but they are very close to each other
- Stainless-steel and Silver spectra

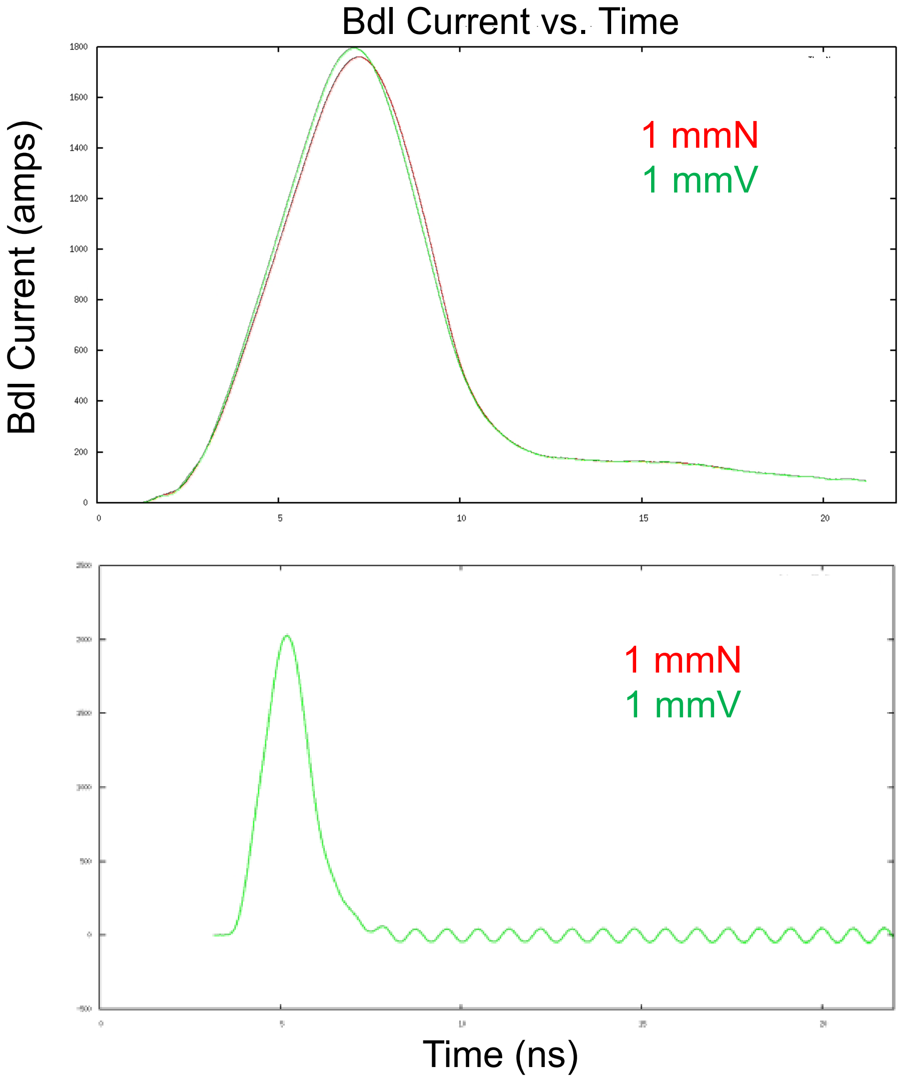
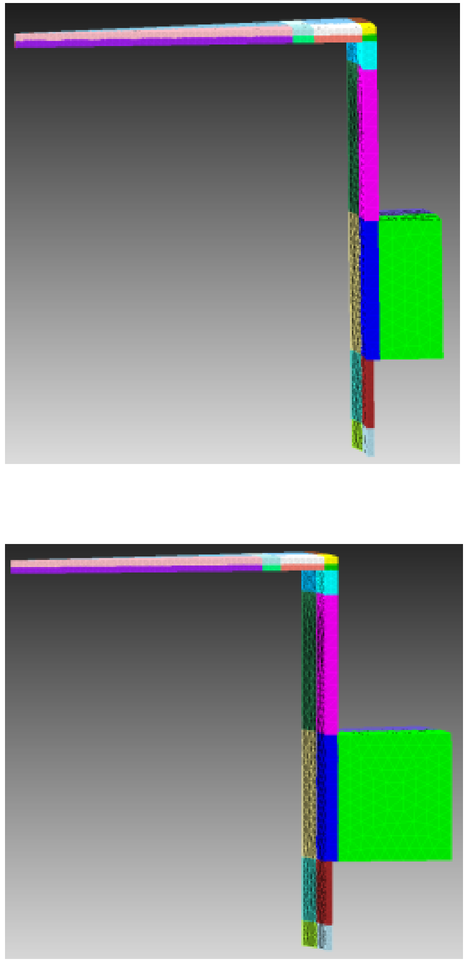
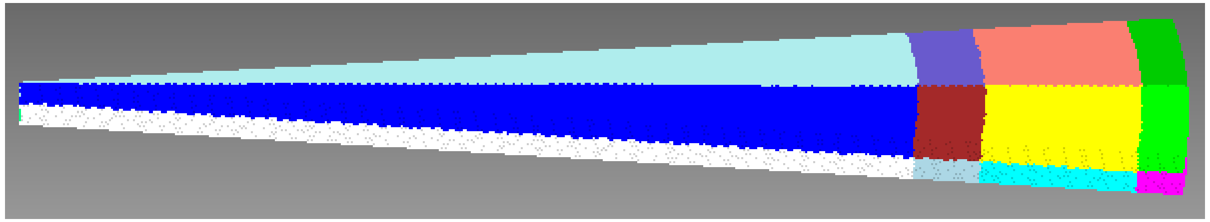


Figure 23: Bdl current vs time for a 1 mmN and 1 mmV Au B-Dot system at vacuum, stainless-steel and silver input spectra

Figure 24: 1 mmV B-Dot full geometry.



1 mm B-Dot Transmission Line Results



- Silver Spectrum
- vacuum

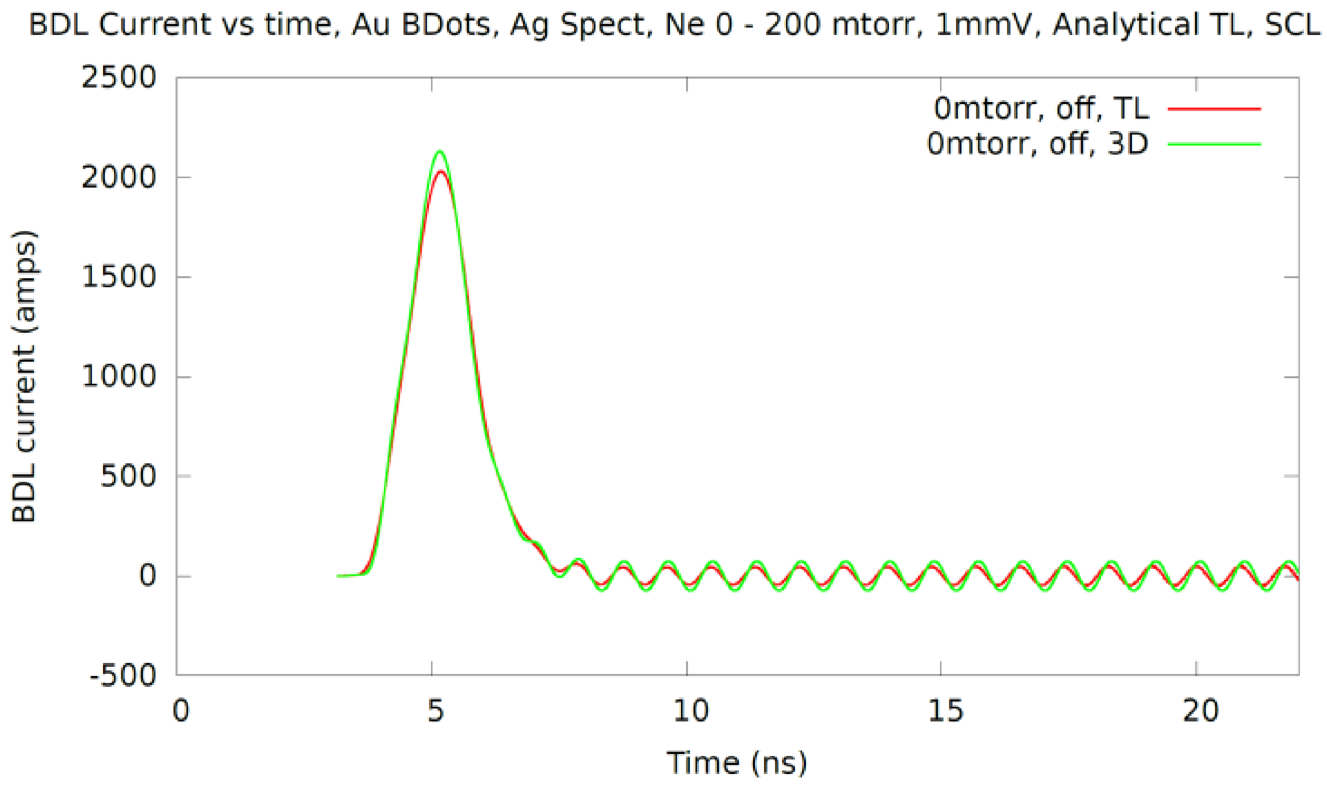
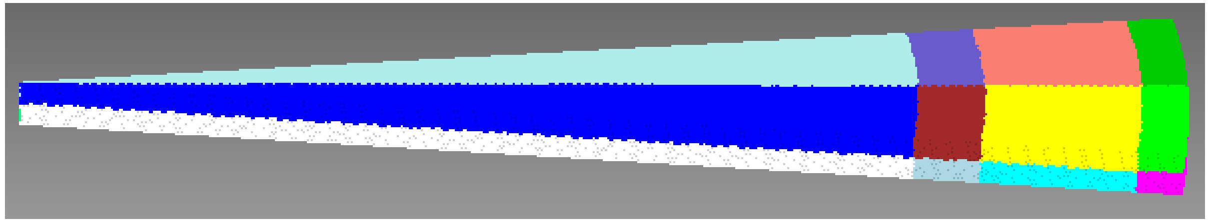
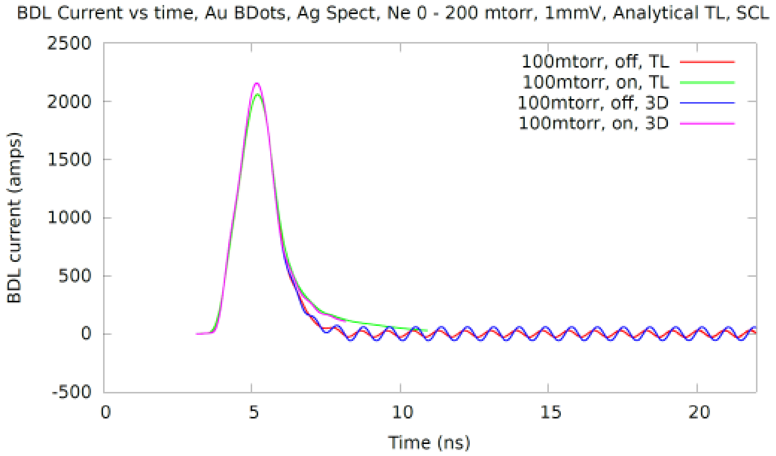


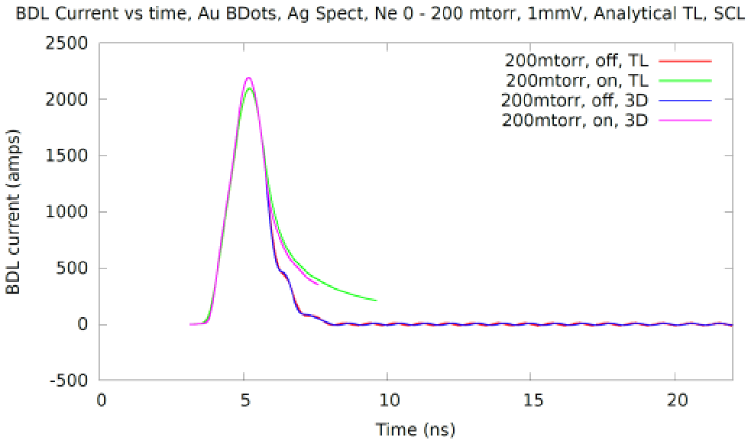
Figure 25: Bdl current vs time for a 1 mmV Au B-Dot system at vacuum, silver spectrum, analytically matched LC

1 mm B-Dot Transmission Line Results



- Silver Spectrum
- Low pressure Ne





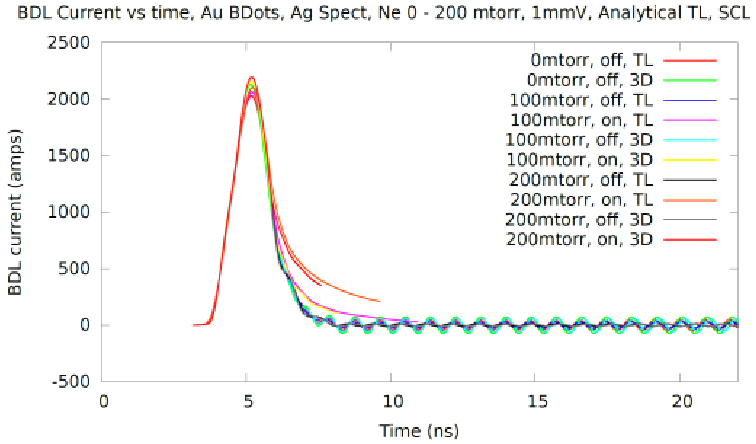
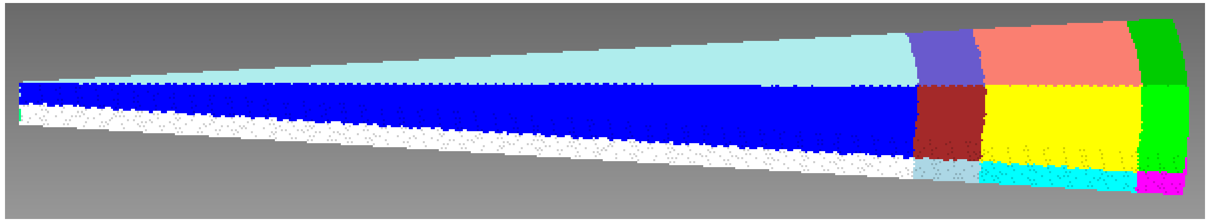


Figure 26: Bdl current vs time for a 1 mmV Au B-Dot system low pressure Ne, silver spectrum, analytic transmission line

1 mm B-Dot Transmission Line Results



- Silver Spectrum
- High pressure Ne

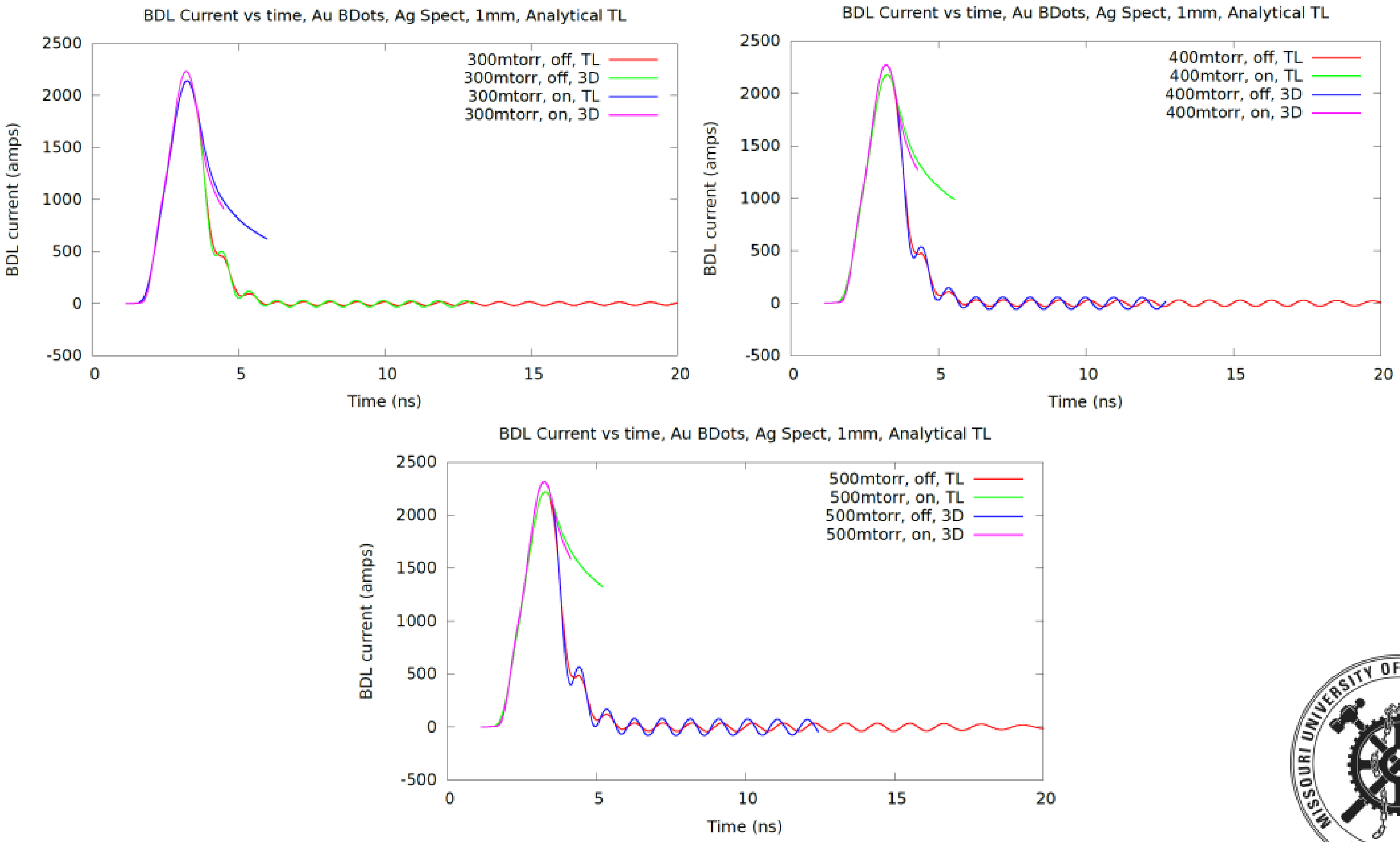
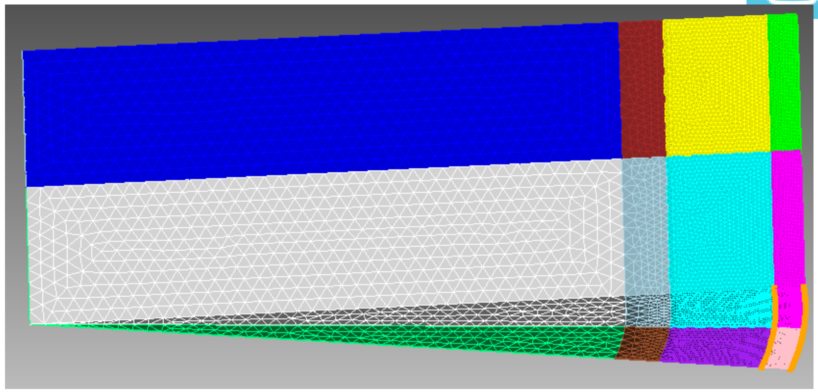


Figure 27: Bdl current vs time for a 1 mmV Au B-Dot system high pressure Ne, silver spectrum, analytic transmission line

10mm B-Dot Transmission Line Results



- Silver Spectrum
- Vacuum
- Analytic Fit

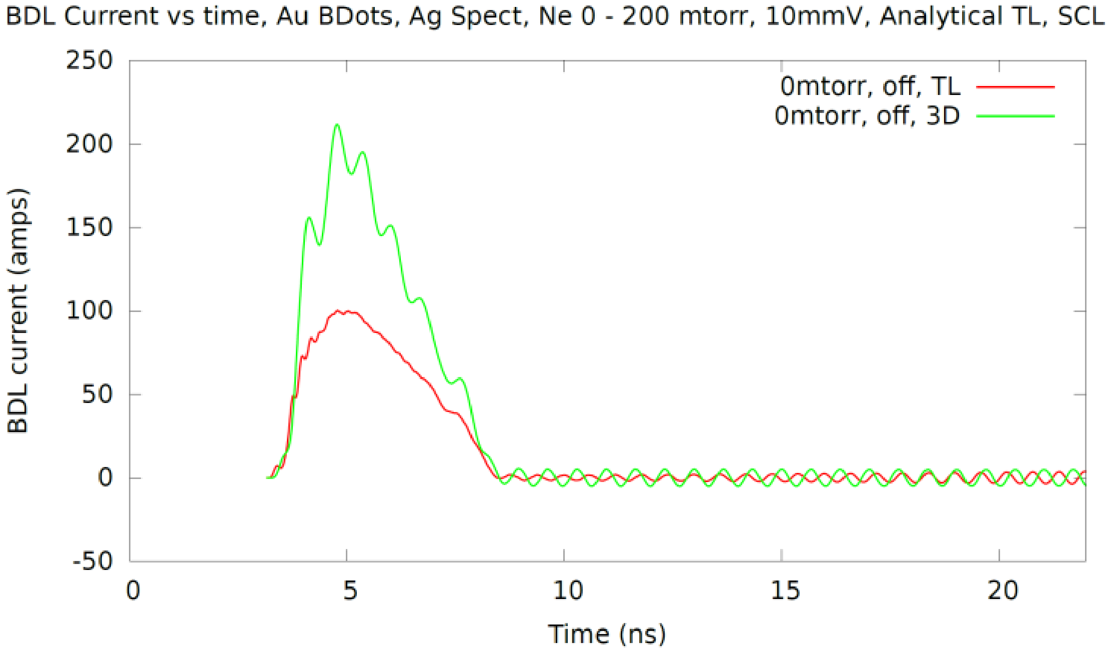
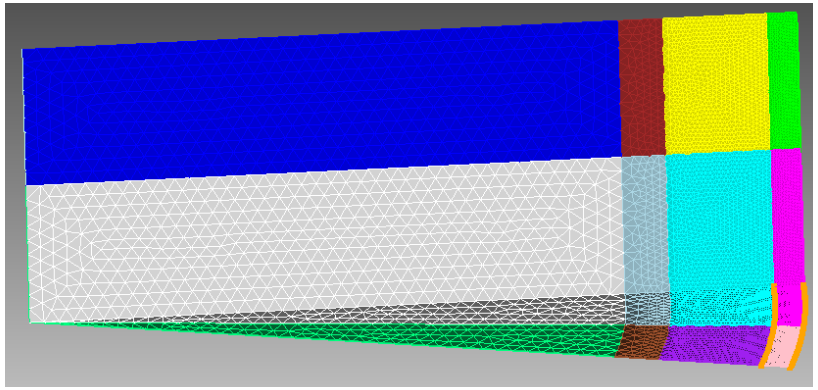


Figure 28: Bdl current vs time for a 10mmV Au B-Dot system vacuum, silver spectrum, analytic transmission line

10mm B-Dot Transmission Line Results

- Silver Spectrum
- Low pressure Ne
- Analytic Fit



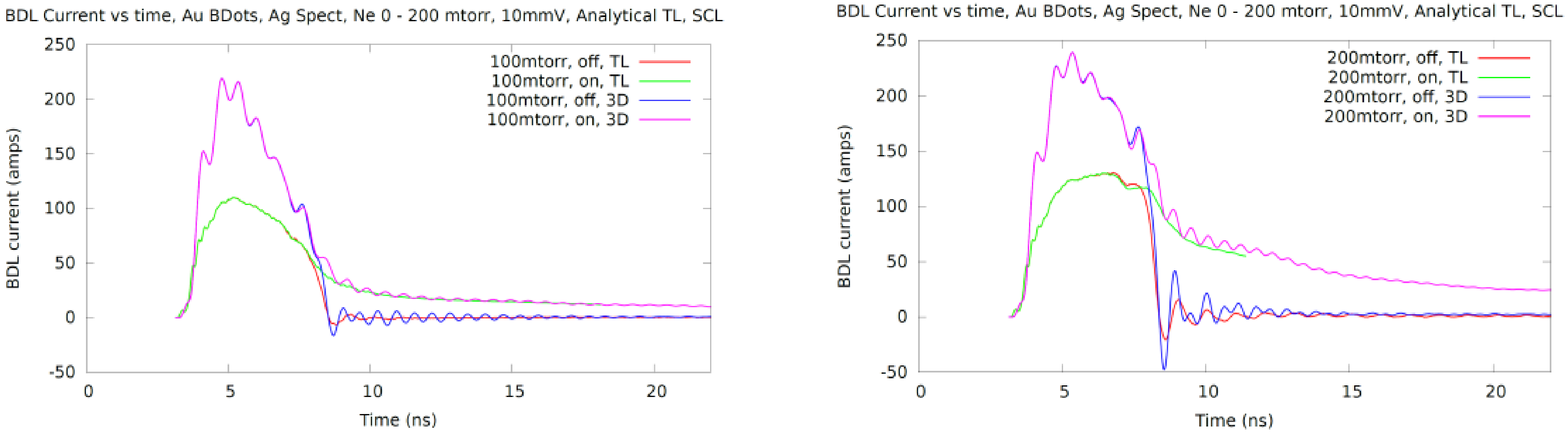
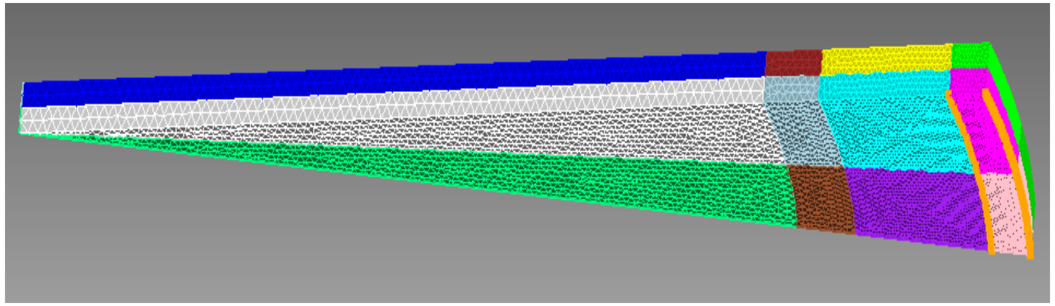


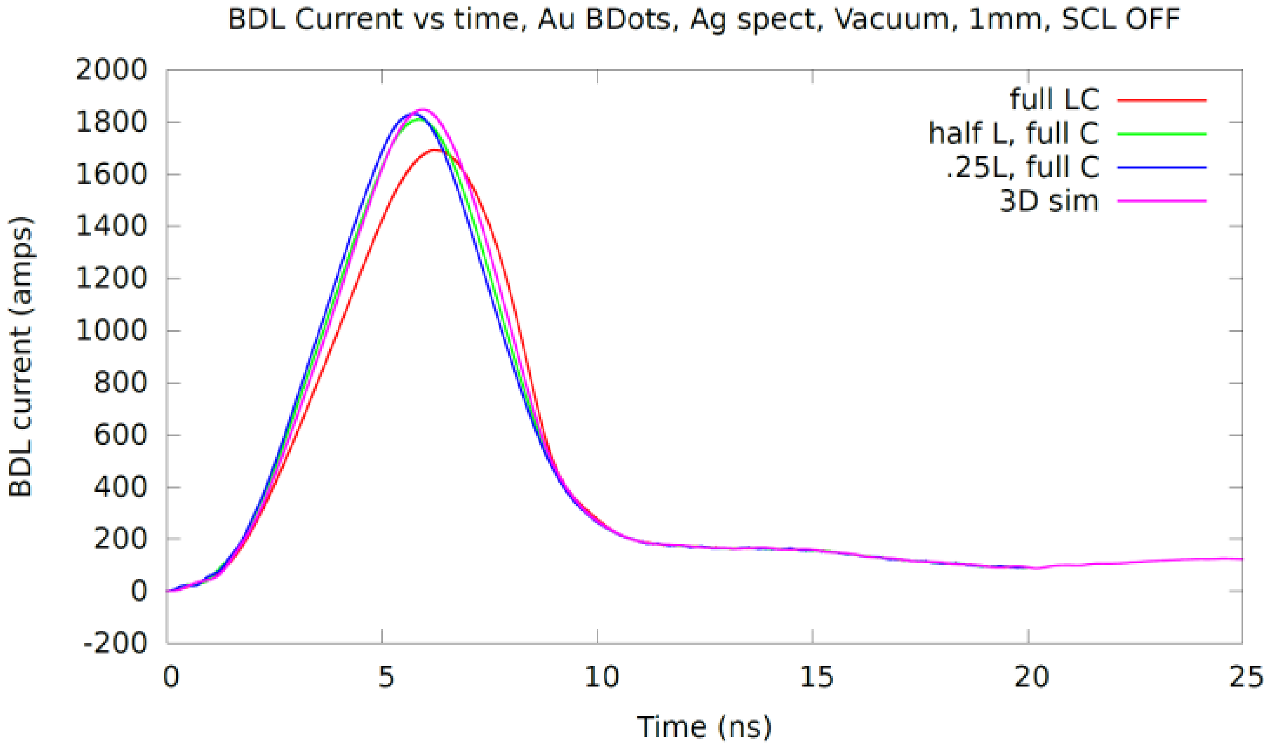
Figure 29: Bdl current vs time for a 10mmV Au B-Dot system low pressure Ne, silver spectrum, analytic transmission line

1 mm B-Dot Transmission Line Results L Comparison

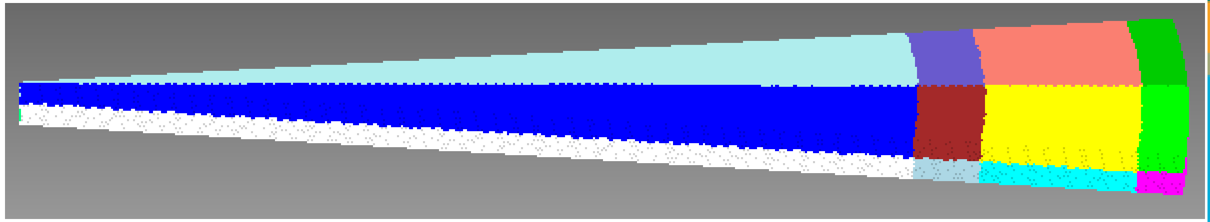


- Stainless-steel input spectrum
- Vacuum
- Calculated LC values in transmission line
- Halving L to match rise-time

Figure 30: Bdl current vs time for a 1 mmV Au B-Dot system at vacuum, stainless-steel spectra, calculated LC values



1 mm B-Dot Transmission Line Results Analytically Matched



- Stainless Steel Spectrum
- Vacuum
- Analytically matched LC values
- Matching rise times, fall times, and oscillation period

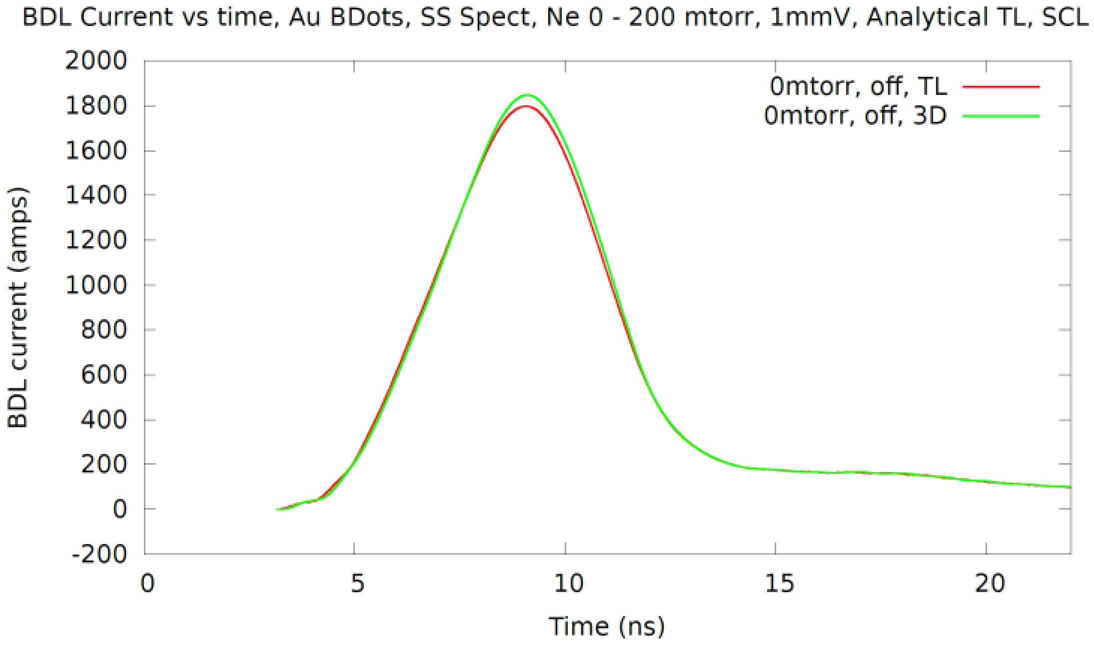


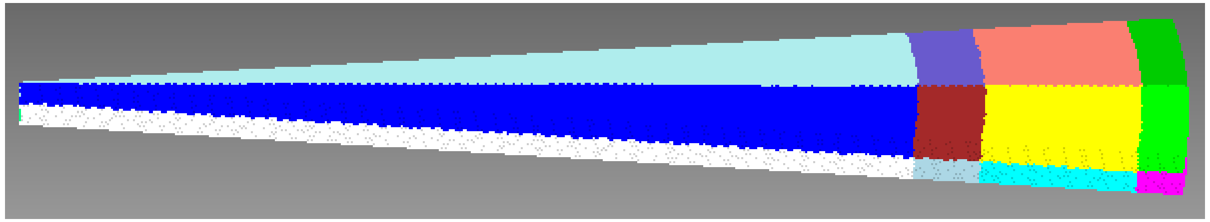
Figure 31: Bdl current vs time for a 1 mmV Au B-Dot system at vacuum, stainless-steel spectra, analytic fit LC values

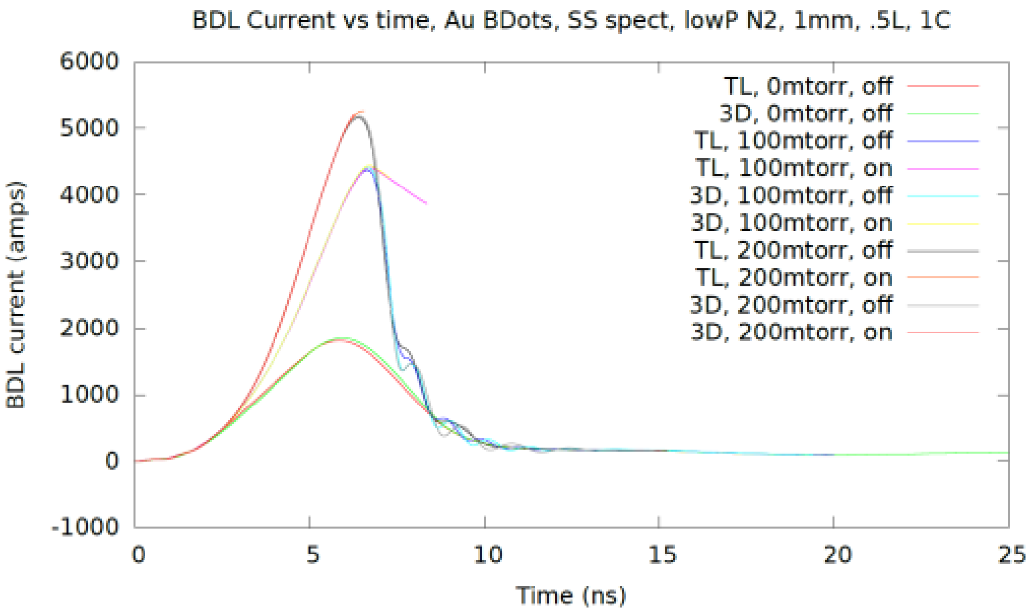
Table 3 Capacitance and Inductances for each section along axial transmission line, analytically fitted LC values

#Length	num_cells	C_l	L_l	G_l
0.002	20	1.003492148e-10	6.852643008e-08	0.0
0.011	110	1.003492148e-10	6.852643008e-08	0.0
0.01	100	1.979256108e-11	3.474322207e-07	0.0
0.005	50	1.987497774e-10	3.459915044e-08	0.0
0.002	20	1.987497774e-10	3.459915044e-08	0.0

1 mm B-Dot Transmission Line Results

- Stainless-steel input spectrum
- Low pressure, N_2 and Ne





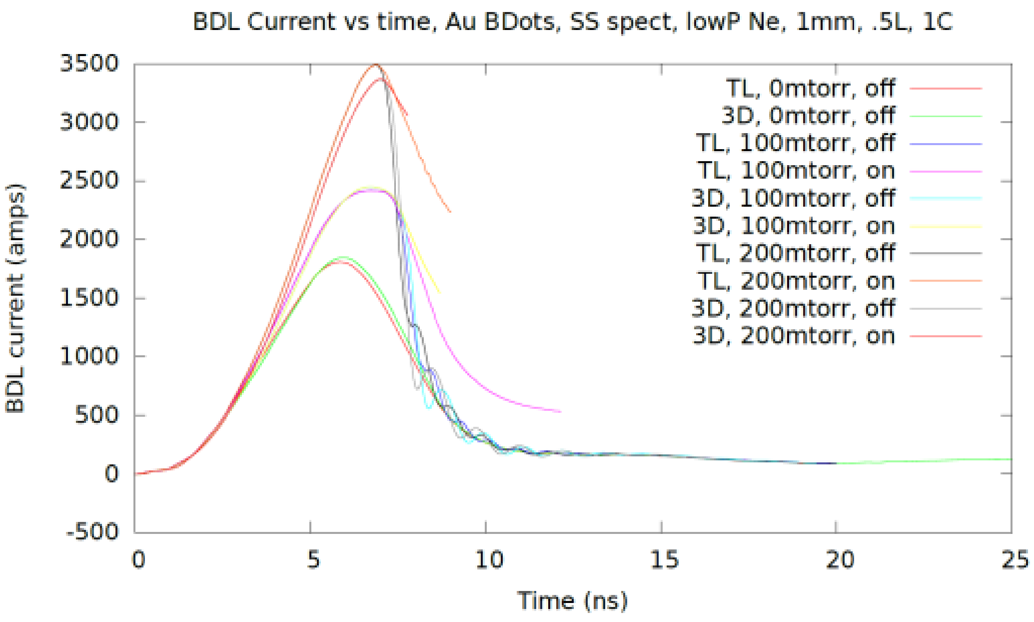


Figure 32: Bdl current vs time for a 1 mmV Au B-Dot system low pressure N_2 (left) and Ne (right), stainless-steel spectra, analytic fit LC values

1 mm B-Dot Transmission Line Results

- Stainless-steel input spectrum
- High pressure Ne
- High pressure N_2 data matches shape, but misses amplitude

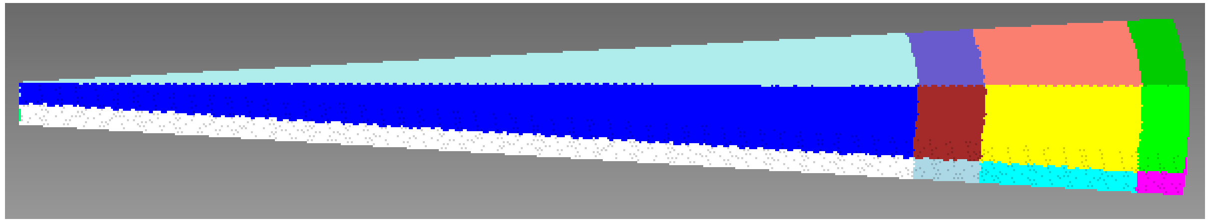
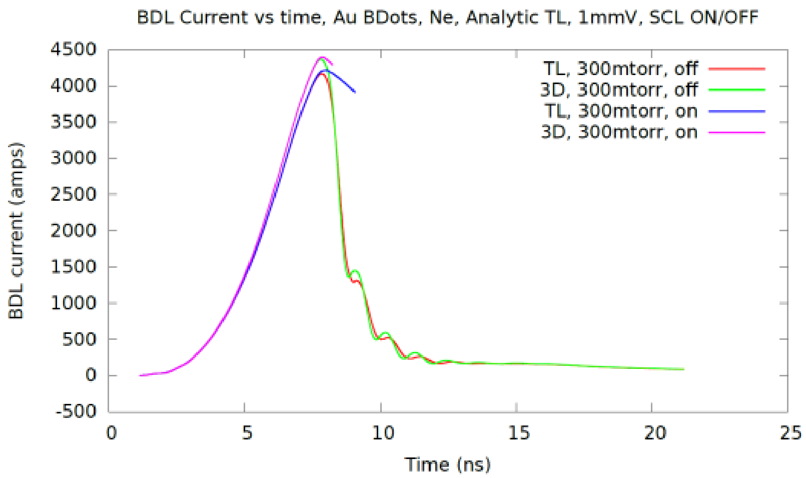
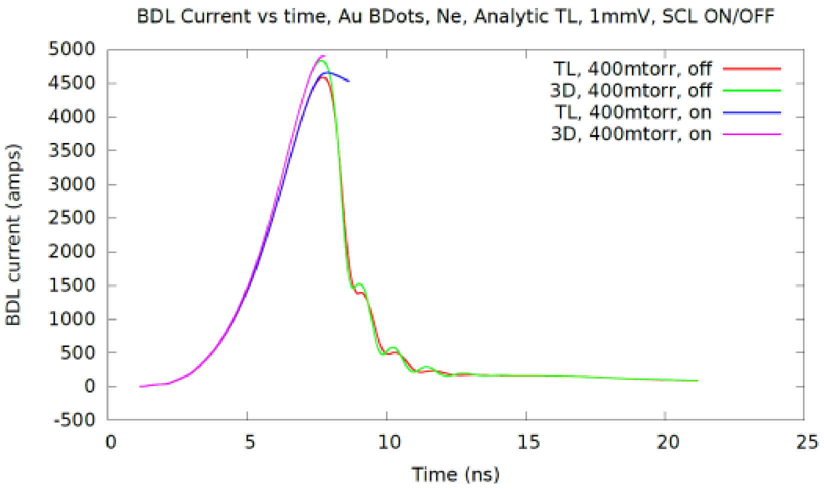
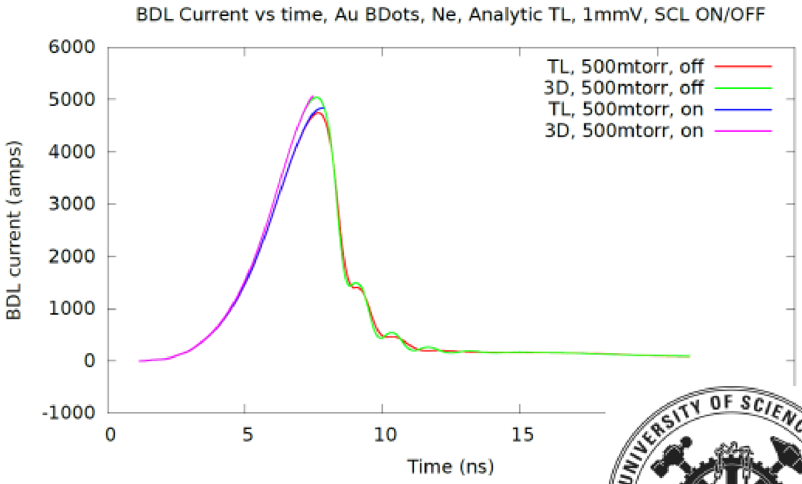


Figure 33: BdI current vs time for a 1 mmV Au B-Dot system with high pressure Ne fill gas, stainless-steel spectrum, analytically matched LC parameters OFF/ON

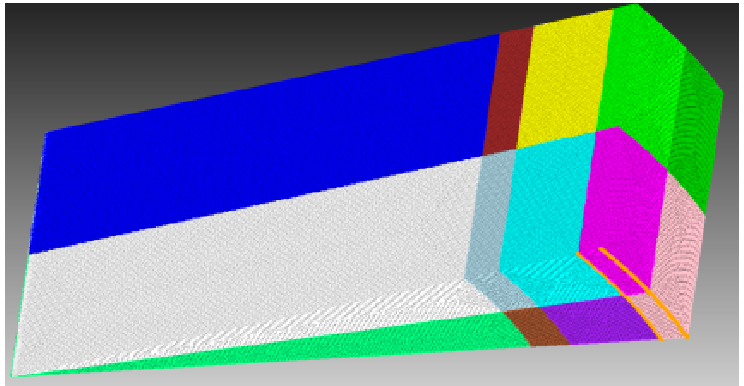


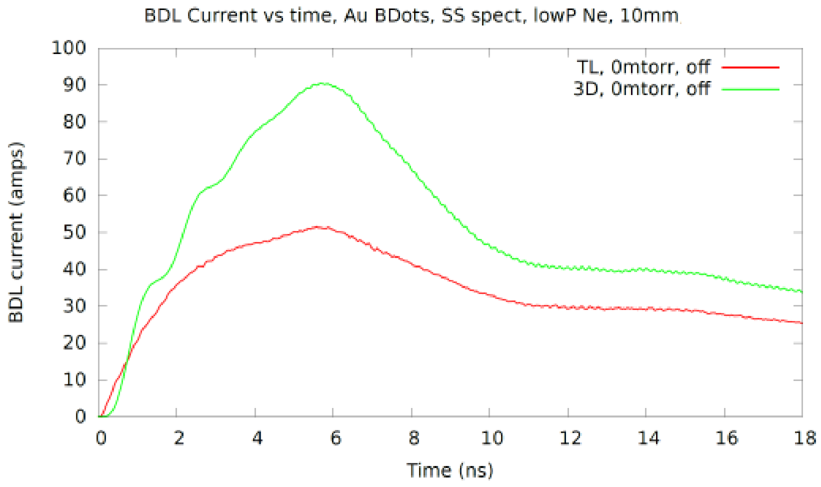




10mm B-Dot Transmission Line Results

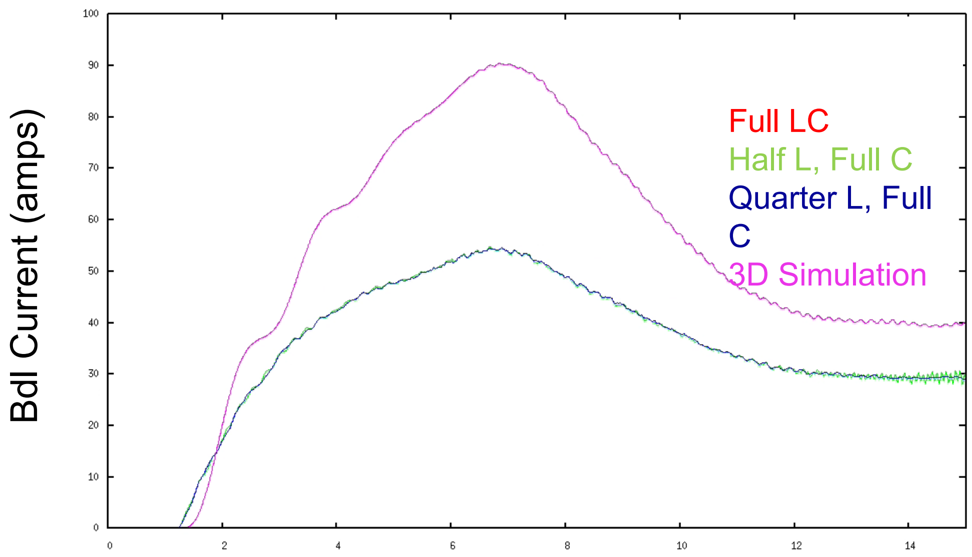
- Stainless-steel input spectrum
- Vacuum





Time (ns)

Figure 34a: Bdl current vs time for a 10mmV Au B-Dot system at vacuum, stainless-steel spectrum, analytically matched LC values

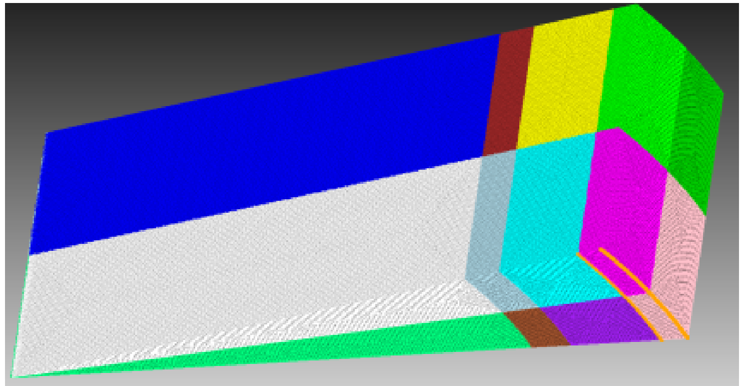


Time (ns)

Figure 34b: Bdl current vs time for a 10mmV Au B-Dot system at vacuum, stainless-steel spectrum, transmission line comparison

10mm B-Dot Transmission Line Results

- Stainless-steel input spectrum
- Low pressure Ne



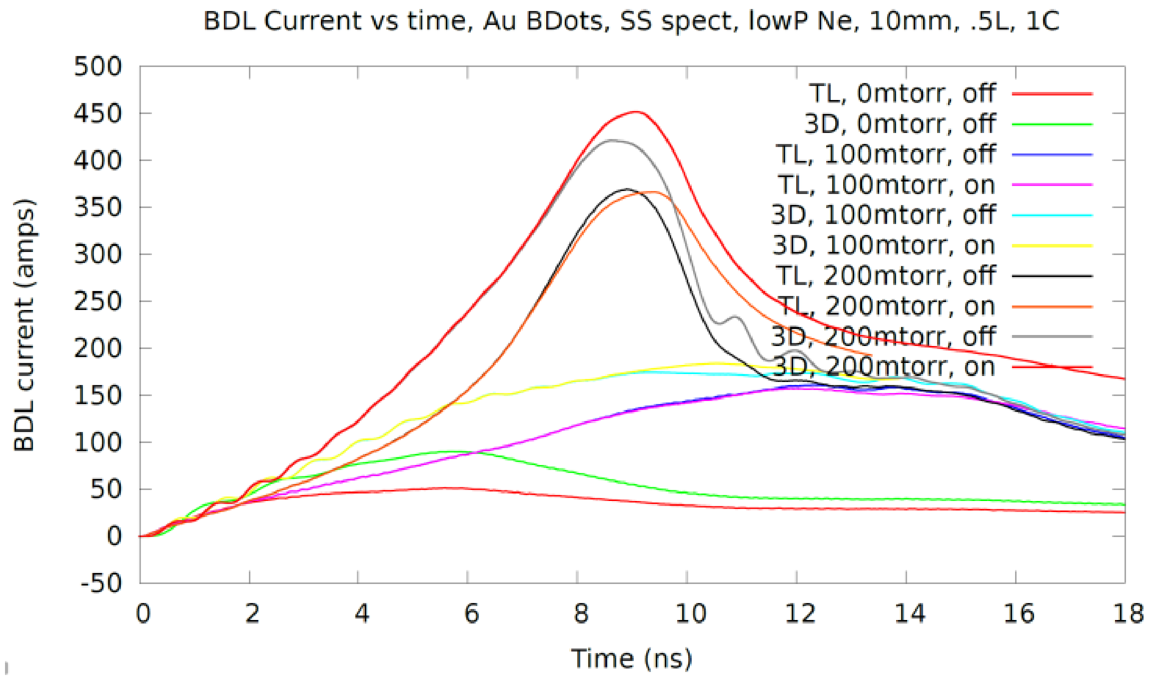


Figure 35: Bdl current vs time for a 10mmV Au B-Dot system low pressure Ne, stainless-steel spectrum, .5L

Outline

- Introduction
- Background Physics
- Methods
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- Discussion
- Conclusion and References
- Acknowledgements and Questions

Discussion: Changing the Diagnostic

- The B-Dot simulation reads Bdl current from one surface photoelectric emission
  - Are there other x-ray diagnostics that are similar to this AK gap simulation?
- XRD-31 – DANTE II
  - National Ignition Facility
    - Different Input spectra are required (Cu, Ag)
  - Photons enter from the top
- Driven AK Gap
  - Modeling a driven LC circuit is much different than an LC circuit that is not driven
  - There is an extra term in the differential equation
  - $\varepsilon_0 = L\frac{\mathrm{d}I}{\mathrm{d}t} + qC$
  - We expect to see different behavior, but modeling it in the EM PIC code is as simple as adding an initial voltage condition to the Circuit block
- The geometry changes with the diagnostic, as well as the boundary conditions, sidesets, and meshing

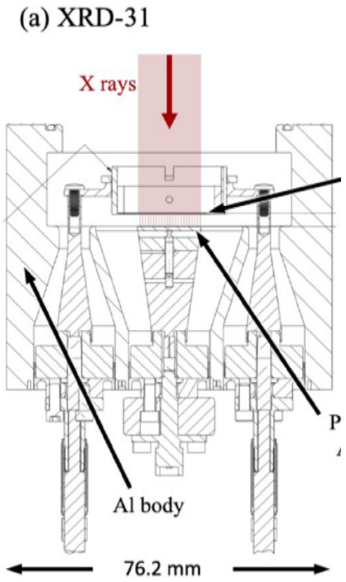

Figure 36: DANTE II XRD build diagram. The puck is being hit by x-rays, and the rest is the external circuit

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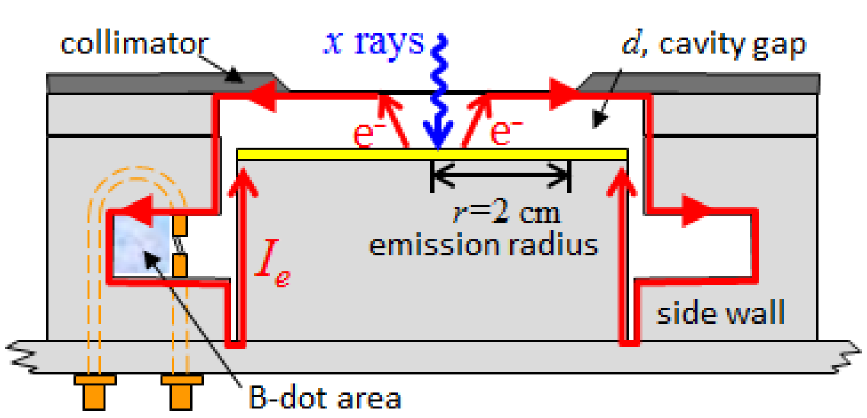
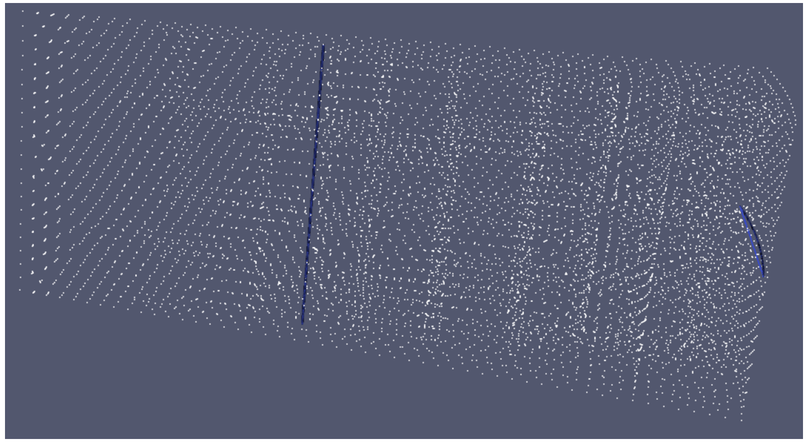
Conclusion

- B-dot current output was simulated for an A/K gap, with a stainless-steel wire array and silver input spectra, an x-ray time pulse and yield from experiment, and a gold irradiation surface
- Coupled MC and EM PIC codes were used to irradiate a surface and measure BdI current in a photoemission driven cavity
- The simulations provide us with a good upper and lower bound of the true expected tail due to SCL emission
- Modeling the edge of the emission cavity as a transmission line is a valid way to analyze this system if the transmission line is brought in axially
- Matching the LC parameters to an analytic fit works for 1 mm gap sizes for both spectra, but fails for 10mm highly space-charge limited cavities
- This method can be used for a variety of x-ray diagnostics

Figure 1





Conclusion

- Future work on this project would be to change the detector to an x-ray diode instead of a B-dot, change the fill gas to Ar, and change irradiation material.
  - Also explore the “why” behind why SCL emission has such a large effect in the 10mm cavities
- The next project for the B-Dot system is to add surface heating post irradiation (Fowler-Nordheim and thermal emission), and see how it effects late time current tail

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Acknowledgements

A special thank you to Peggy Jo Christenson, Keith Cartwright, Adam Darr, and Scot Swan for helping me with the simulations and physics, and for being great mentors. I'd also like to thank Tim Flanagan for providing the time pulses, experimental data, x-ray yield data, and input photon spectrum and Sandia for providing the computational resources. A final thank you goes to my advisor, Dr. Ayodeji Alajo and my committee members, Dr. Syed Alam and Dr. Joseph Graham.

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Simulating LC Circuits in Cylindrical Photoemission Driven Cavities Using Coupled Monte Carlo and Particle-in-Cell Codes

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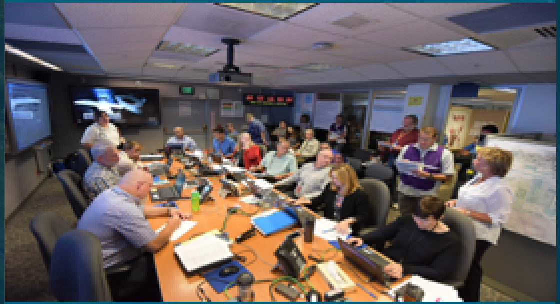

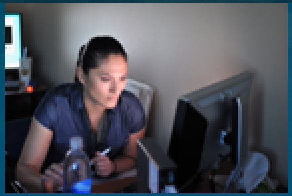

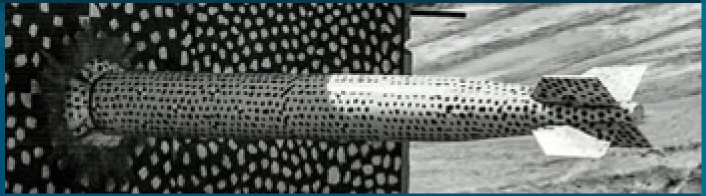

Questions?

Thanks!

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[2] Missouri University of Science and Technology: Nuclear Engineering and Radiation Sciences

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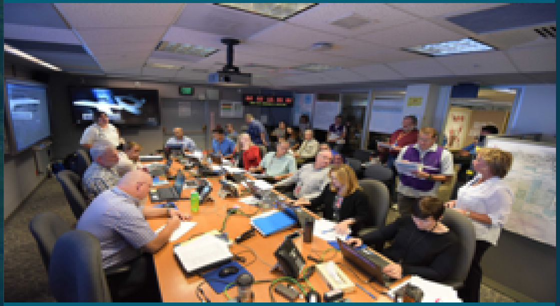
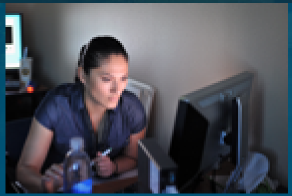
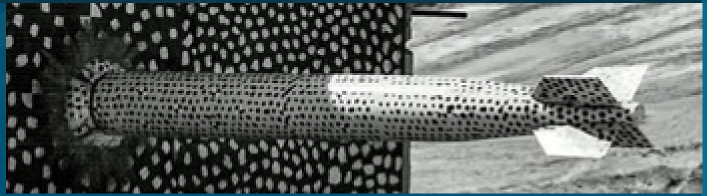
Simulating LC Circuits in Cylindrical Photoemission Driven Cavities Using Coupled Monte Carlo and Particle-in-Cell Codes







EXTRA SLIDES

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[2] Missouri University of Science and Technology: Nuclear Engineering and Radiation Sciences

Introduction

There are two parts to the simulation

- Monte-Carlo Stochastic photon/electron transport code **(MC photon/electron code)**
    - Generates a photoelectron emission spectrum for each emission surface
    - For this experiment, the transport code requires an input photon spectrum
        - **Stainless-Steel Z-Pinch Wire Array for these shots**
    - The photoelectron emission spectrum, an x-ray time pulse, and yield are used to characterize electron emission in the gas filled cavity
- Electromagnetic kinetic Particle-in-Cell plasma physics code **(EM PIC)**
    - Solves coupled Maxwell's equations in the presence of charged particles to self-consistently model the electromagnetic plasma dynamic evolution within the AK gap
    - Outputs include total charge, **Bdl current**, Edl voltage, and field strengths

HPC Cluster at SNL

Photoelectric Effect

- A metal is irradiated with photons
  - E_{ph}= hv
- Electrons are emitted
  - This creates a current
- Emission corresponds to energy of the photons
  - Materials have “resonances” where most of the photoemission occurs
- Helped prove that photons and quantized [4]
- **The simulation uses a spectrum of photons, not a monoenergetic source**
  - Example sources include SS, Cu, Ag, Mo, Kr in the X-Ray range
  - Z machine and NIF spectra

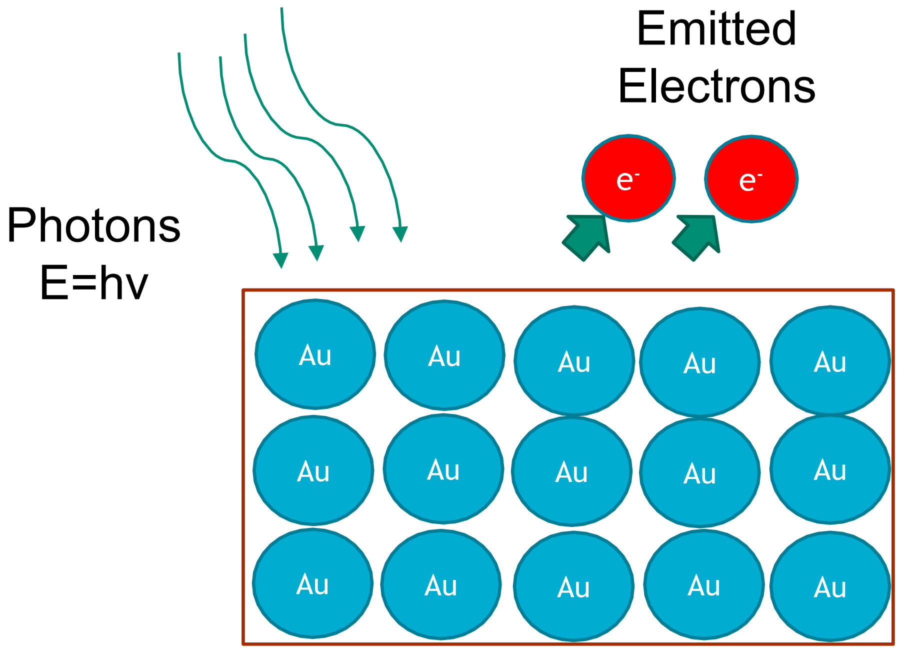


Figure 2: Photoelectric effect animation. Not to scale

Child-Langmuir Law: Space-Charge Limited Emission

- Picture a parallel plate capacitor infinite in x and y with height d, and charge Q
  - Q=CV $Q_{||plate} = AV\varepsilon_o/D$ $v_{max} = (2eV/m_e)^{1/2}$ J = I/A
  - C is capacitance, V is voltage, A is area of the plate, D is gap size
  - v_{max} is max velocity, ε_o is permittivity of free space, e is electric charge, m_e is mass of an electron
  - J is current density, and I is current
- The average velocity of the (non-relativistic) electrons across the gap is half of the maximum velocity
  - The current across the gap can be written as $I = Q\bar{v}/d$
  - Therefore, we get equations 3 and 4
- **Our simple derivation gets us very close to the Child-Langmuir law and provides us with a simple picture of SCL emission effects**
  - The difference comes from our assumption that the average electron velocity is half of the maximum velocity

$$J_{CL} = \frac{4\epsilon_0}{9}\sqrt{\frac{2e}{m}}\frac{V^{3/2}}{d^2}. \quad 1$$

$$\bar{v} = \frac{v_{max}}{2} \quad 2$$

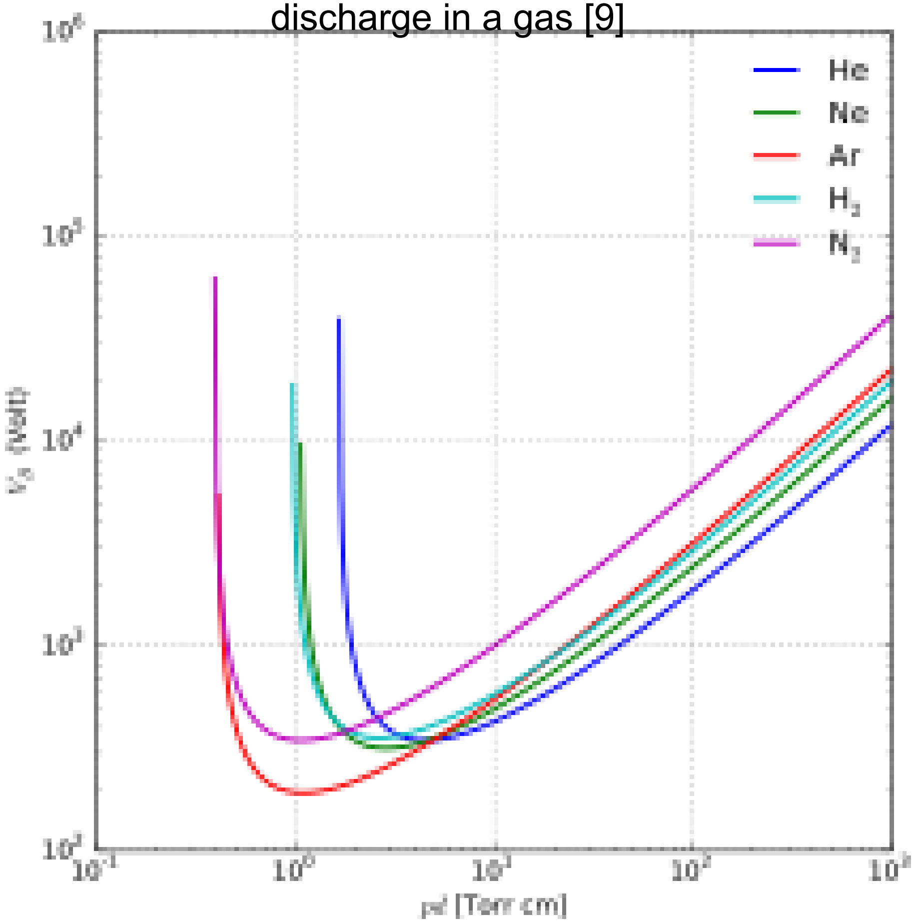
$$I = \frac{\epsilon_0 AV}{2D^2}\sqrt{\frac{2eV}{m}} \quad 3$$

$$J = \frac{\varepsilon_0}{2}\sqrt{\frac{2e}{m_e}}\cdot\frac{V^{3/2}}{D^2} \quad 4$$

Gas Ionization and Paschen Curve

- In the cavity, energy required for electric discharge is a function of pressure and gas species
- As more plasma is generated by photoelectron emission, Bdl current (current induced in the B-dot) should increase
- However, the **Paschen curve** tells us there is a minimum energy required to ionize different fill gases [9]
- More energy is required for ionization after the fill gas pressure exceeds minimum pressure
- Current vs. pd: peak current increases to a maximum, and then decreases

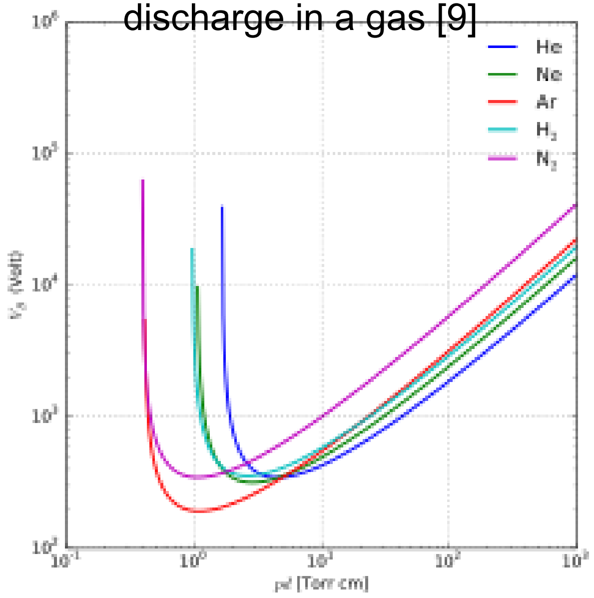
Figure 2: Paschen Curve for many gasses. The x-axis is pressure (torr) per cm, and the y-axis is energy (volts). This is the energy required for electric discharge in a gas [9]



Gas Ionization and Paschen Curve

- We will see almost an inverse Paschen curve, where instead of voltage decreasing to a minimum and then increasing as a function of pressure, the current increases to a maximum and then decreases as a function of pressure
- This work will focus on Ne (a noble gas) and N_2 (diatomic molecules)
  - Based on the curve, we expect the maximum current of an N_2 filled cavity to peak at lower pressure than Ne
- The form for the Paschen curve is given by equation 5 [7]
  - V is voltage, p is pressure, d is gap size, γ_{se} is the secondary electron emission coefficient, A is the saturation ionization coefficient, and B is the coefficient related to the ionization energy of each gas

Figure 2: Paschen Curve for many gasses. The x-axis is pressure (torr) per cm, and the y-axis is energy (volts). This is the energy required for electric discharge in a gas [9]



$$V_B = \frac{Bpd}{\ln(Apd) - \ln\left[\ln\left(1 + \frac{1}{\gamma_{se}}\right)\right]} \quad 2$$

Background Information

Other things to look at in this simulation

- Convergence testing of the stochastic photon/electron code
- Edl Voltage (voltage in the cavity)
- Other irradiated materials (Ni, Ti, Ag)
- Different input spectra (Cu, Ag)
- Changing the cavity height to 1 mm (reduces SCL emission)
- Fluence scanning
  - Changing the distance from the source to the irradiation surface
- Different filter stacks
  - Materials and thicknesses

Monte Carlo Methods

- Random Sampling to mimic complex systems [11]
  - Monte Carlo **(MC)** methods are useful when the analytic solution is not easy to write
- A general pattern for MC simulations is to model a system as a series of Probability Density Functions (PDFs), sample from the PDF many times, and tally the results
- Random number corresponds to a value in the PDF
- Tracks particle until it leaves system or "dies"
  - Each event corresponds to a physical event (emission, absorpti
- Tally results, and repeat process for many particles
  - The spectra generated in the methods used >10^9 particles

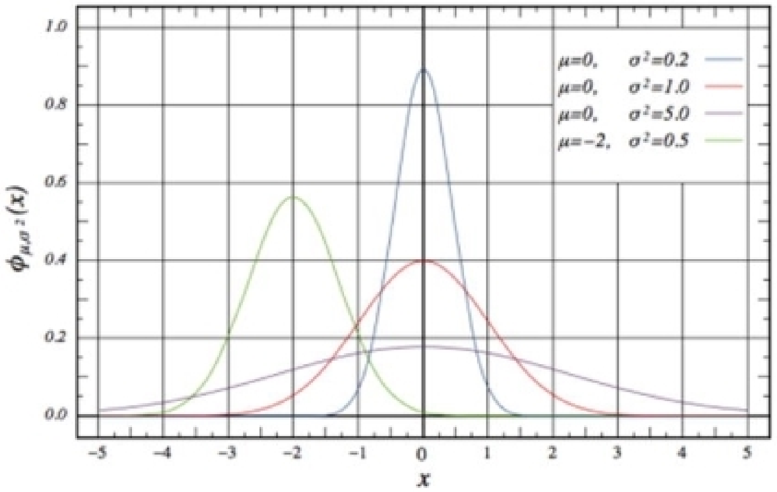
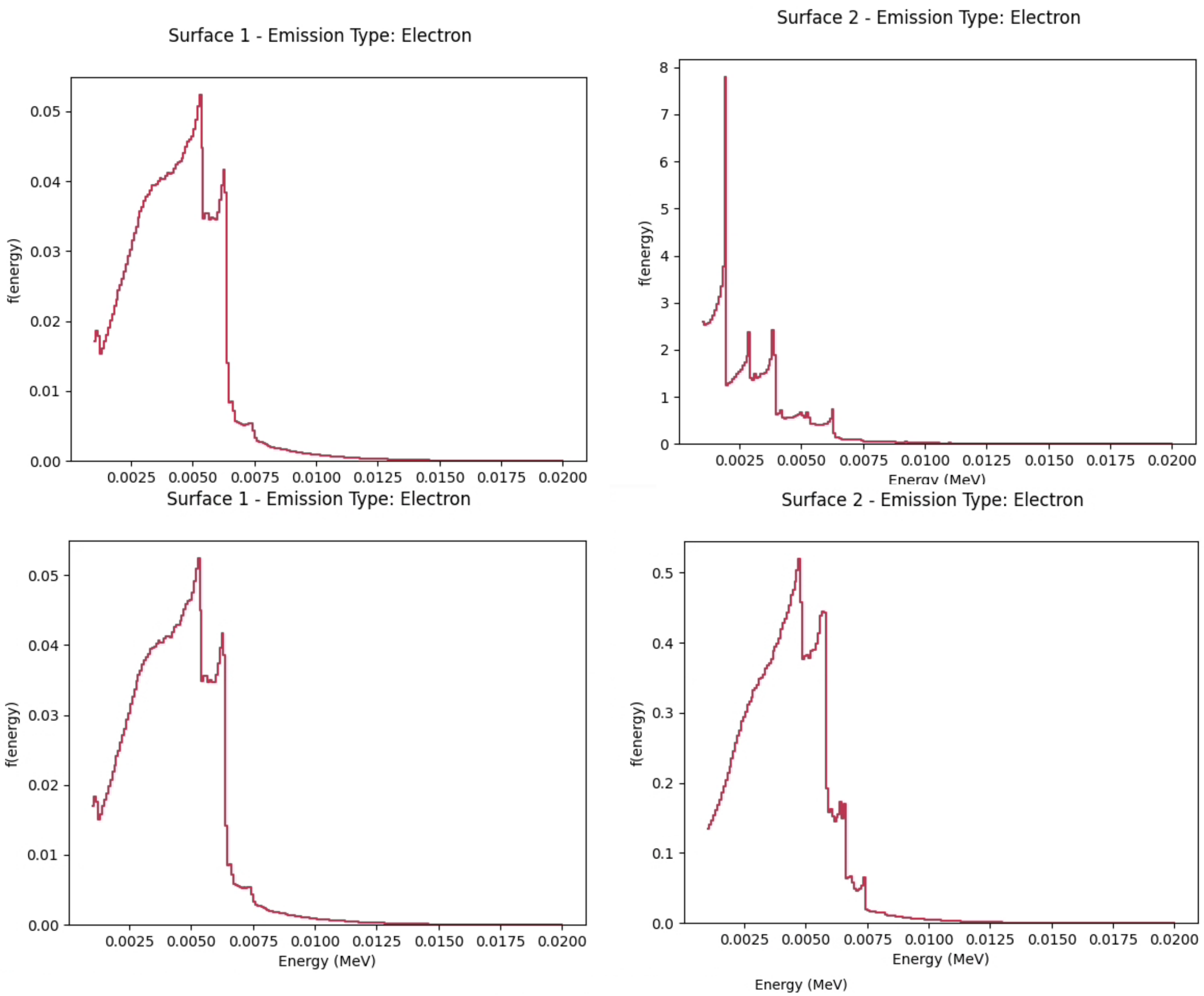


Figure 4: Gaussian distribution with different standard deviations and average values created by an MC method [11]

Monte Carlo Photon/Electron Code: Photoemission Driven Cavities Input Spectra



Gold Puck

Nickle Puck

Figure 5: Photoelectron emission spectra for stainless steel x-ray source from the anode (left) and cathode (right) surfaces. The x-axis is energy in MeV, and the y-axis is emission at the given energy bin. At 5keV, the emission peaks in the top surface; however, this is still much lower emission than the bottom surface at the same energy. Therefore, the bottom surface (gold) is the dominant emitter for this system

Monte Carlo Photon/Electron Code: Photoemission Driven Cavities Input Spectra

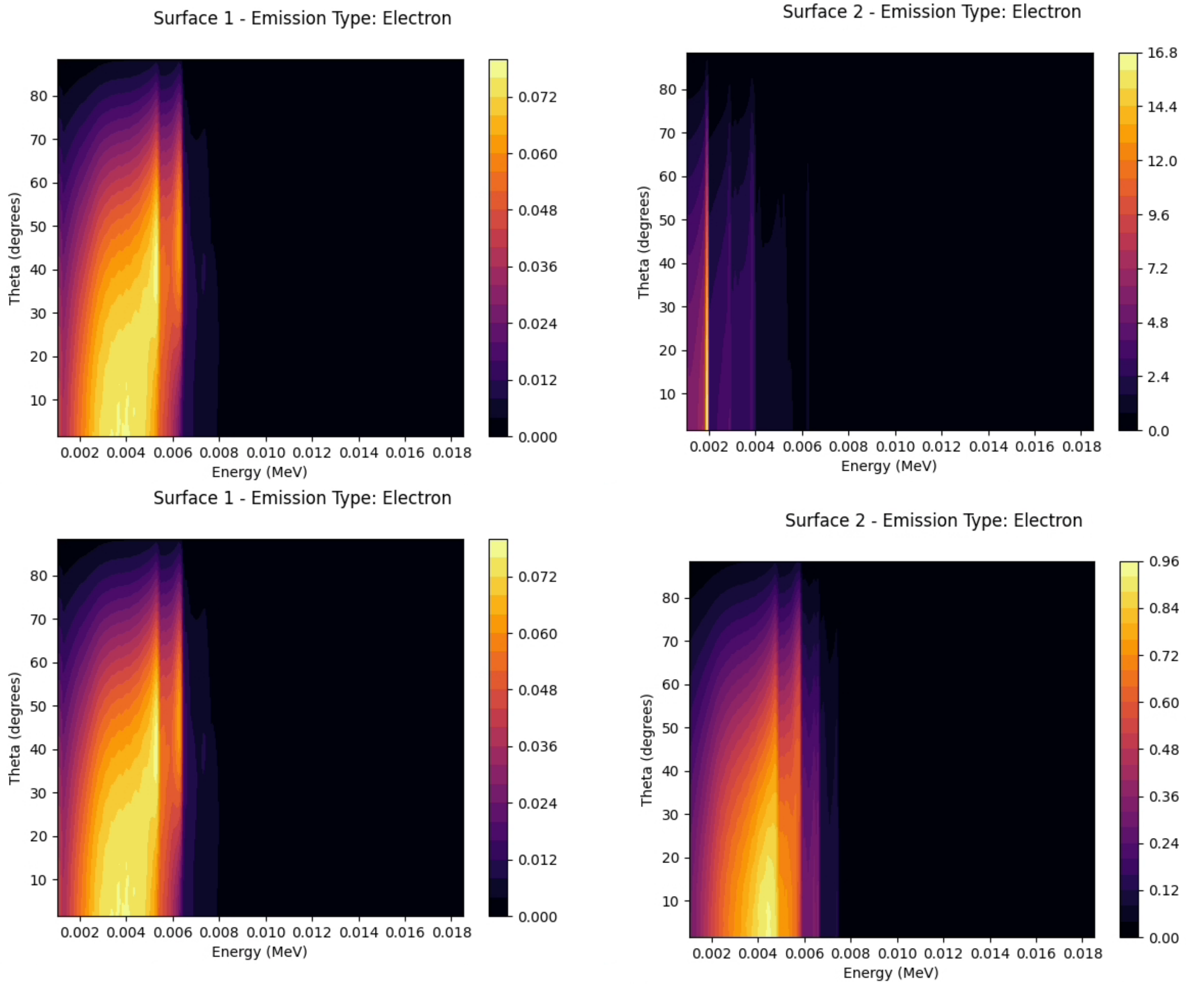


Figure 4: Photoelectron emission spectra for Au from the anode (left) and cathode (right) surfaces. The x-axis is energy in MeV, and the y-axis is emission at the given energy bin. At 5keV, the emission peaks in at the top surface; however, this is still much lower emission than the bottom surface at the same energy. Therefore, the bottom surface (gold) is the dominant emitter for this system

Convergence Testing

- The number of histories in the MC photon/electron code changes the photoelectron spectrum
- More histories is better until a point of diminishing returns (solution converges)
- There is an uncertainty associated with each energy bin
- Bins are sorted by energy and azimuthal angle as shown
  - The first column is energy bin in MeV, the 2^{nd}, 4^{th}, and 6^{th} columns are photoelectric emission at a given angle, and the 3rd, 5^{th}, and 7^{th} columns are the uncertainty associated with the calculation
    - Lower uncertainty is better
- This particular output file was for a stainless-steel spectrum incident upon gold, with 10^8 particles (histories)

Table 1 MC photon/electron code data showing uncertainty in each energy and theta bin

ENERGY INTERVAL (MEV)						
2.000E-02 - 1.700E-02	8.07E-06	3	7.82E-06	3	7.72E-06	3
1.700E-02 - 1.692E-02	2.57E-05	10	1.77E-05	12	1.92E-05	12
1.692E-02 - 1.684E-02	2.89E-05	10	2.72E-05	10	2.28E-05	11
1.684E-02 - 1.676E-02	2.54E-05	10	2.59E-05	10	2.36E-05	10
1.676E-02 - 1.668E-02	3.14E-05	9	3.11E-05	9	2.56E-05	10
1.668E-02 - 1.660E-02	2.89E-05	10	3.01E-05	9	2.46E-05	10

Circuit Modeling

- Changing the relative permittivity (ε_r) will change the value for L and/or C, as shown below
  - $c = \frac{1}{\sqrt{LC}}$
  - $c = \frac{1}{\sqrt{\mu_0 \varepsilon_0 \varepsilon_r}}$
- Therefore
- $\varepsilon_r = \frac{LC}{\mu_0 \varepsilon_0}$
- However, the EM PIC code fixes inductance and varies capacitance. This is the opposite of what we want, as the LC ringing is more of an inductive effect than an capacitive effect.
- L and C were computed by the code

Table 2 Important parameters for circuit modeling, including L,C, and geometric parameters

Inductance (nH)	.620
Capacitance (nF)	.058
Transmission line boundary (mm)	25
Cavity Height (mm)	10
Transmission Line Length (mm)	30

Conversion Testing

- Comparison to emission spectrum of a 6 billion history stainless steel x-ray spectrum to less converged solutions
- The bottom emitter is gold, the top emitter is Al + C
- The legend is the number * 1 million
  - .5 = .5million
- More variance at lower energies
  - Most of the photoelectrons are here, so it is important to have a well converged spectrum at low energies
- Many of the emission values are between .1 and .001, so a difference of .01 or higher is very significant
- Restarting the simulation at various history numbers was essential to running this problem 2 or 3 times, instead of 13+ times

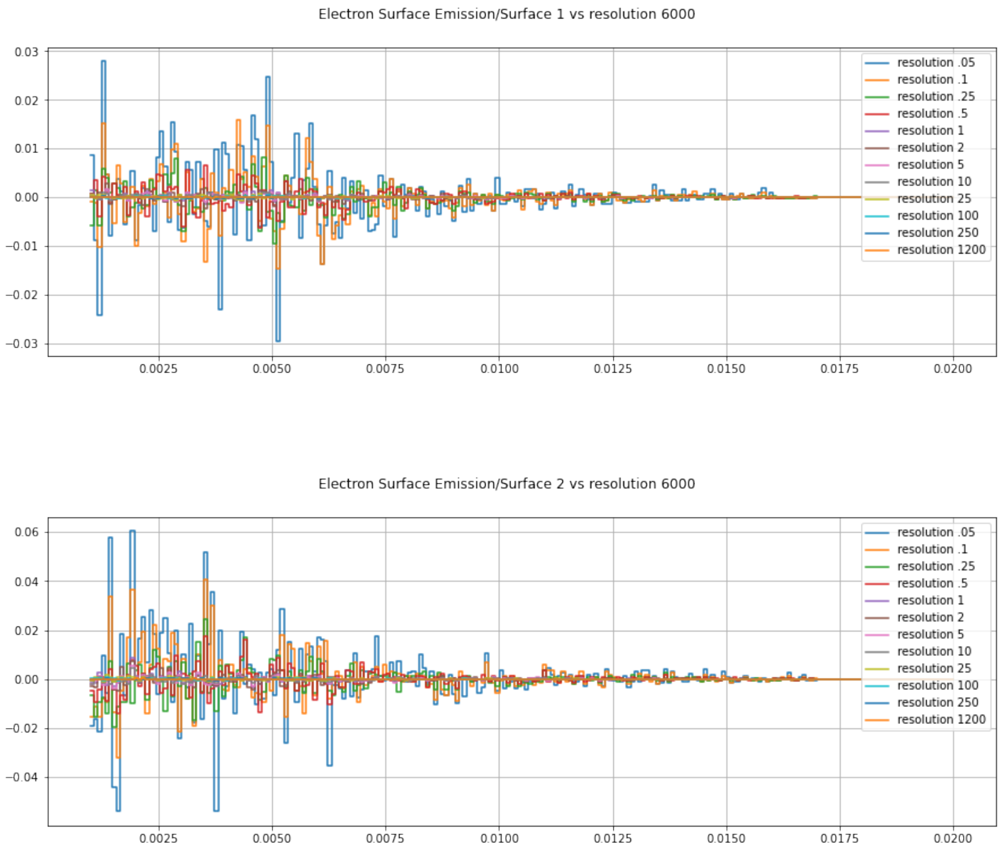


Figure 15: Difference in intensity compared to a 6 billion history simulation for less converged 10mm Au B-Dots

Converging Testing

- The sigma cumulative density function (CDF) is easier to read and understand
- Look at the 10 million particle line (black, surface 2)
  - The CDF tells us that 80% of the energy and theta bins have uncertainties less than 20%, where lower is better
  - We can see clear convergence as histories increase
- The goal is to have as many uncertainties under 10% as possible
- For surface one, the 1.2 billion particle CDF has less than 5% of the particles with an uncertainty greater than 10%
- The point of diminishing returns for surface 2 is closer to 250 million histories, where 5% of the uncertainties are greater than 10%

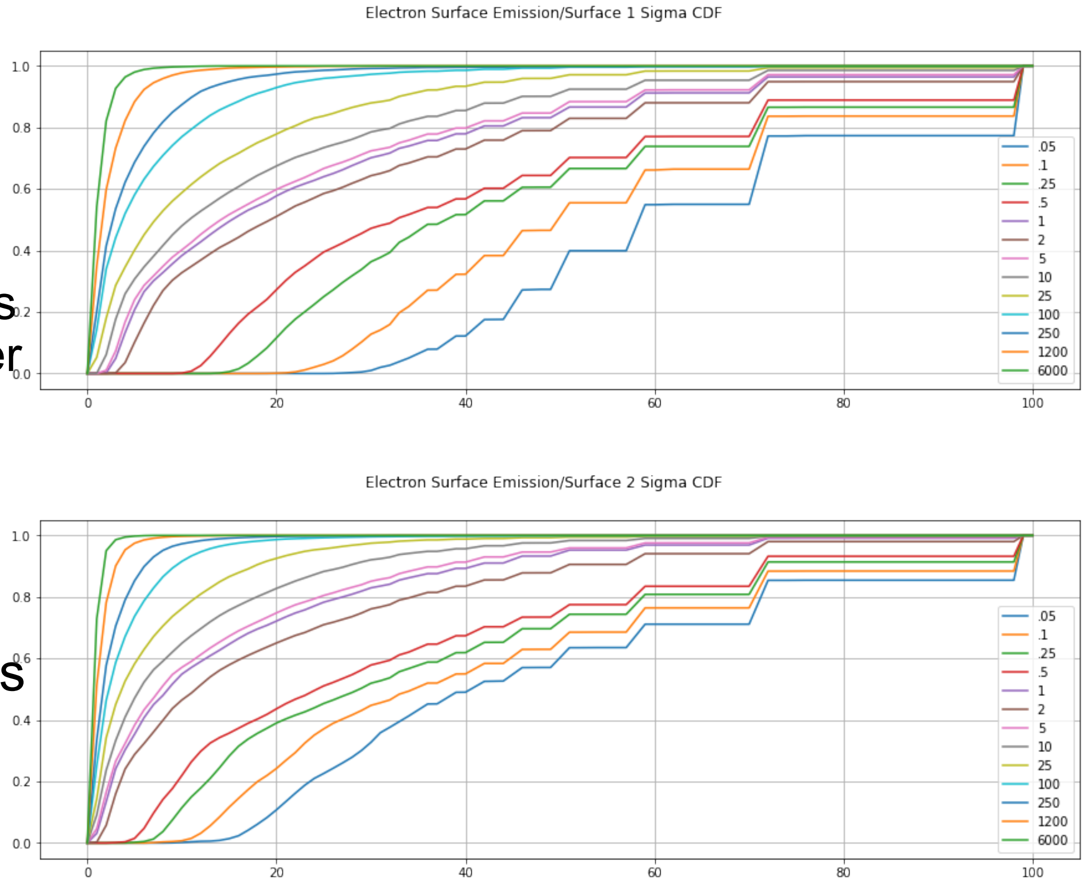
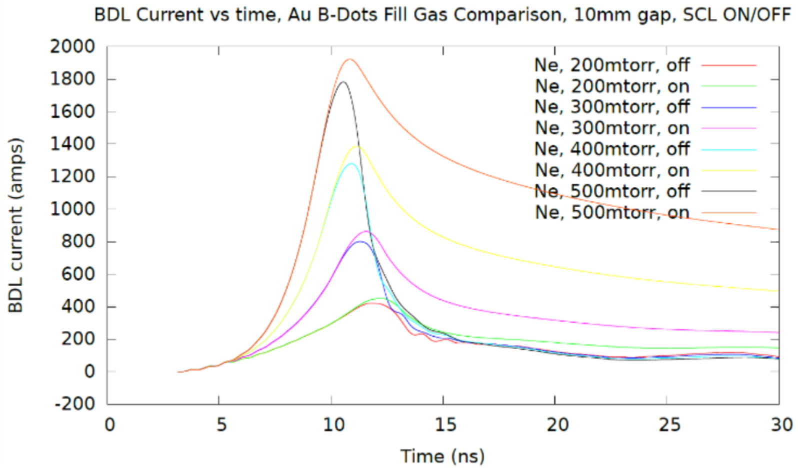
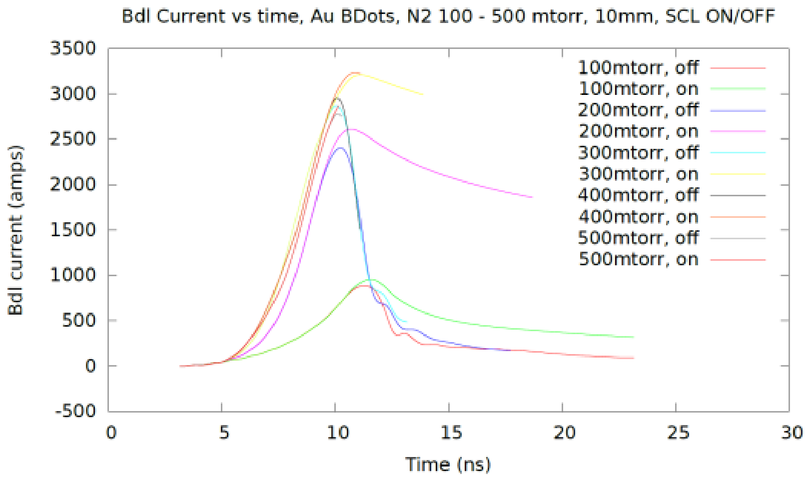


Figure 16: Uncertainty CDF for different number of histories for 10mm Au B-Dots

N_2 and Ne Fill Gas Comparison, High Pressure

- Ne's peak current occurs at 500 mTorr (on/off), and increases until this point
- N_2's peak current occurs at 300 mTorr
  - This means that around 300 mTorr correlates to the minimum in the Paschen curve
- As pressure increases, the current rise time decreases
- From Figure 15b, we see that the peak current for Ne is much higher before SCL emission effects and electric discharge effects take place
  - N_2 peaks earlier than Ne in every case





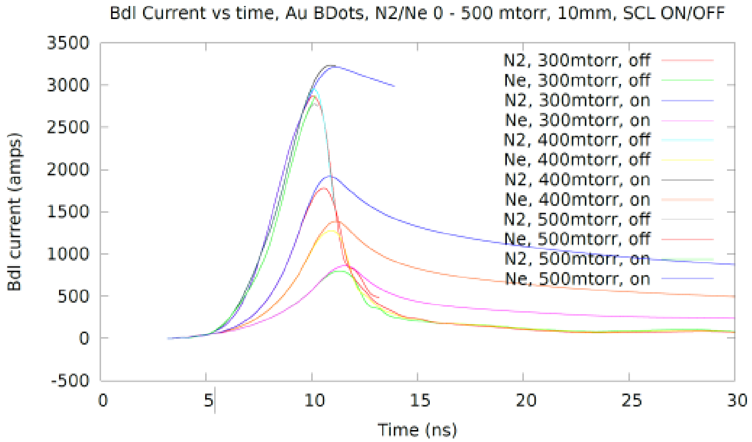
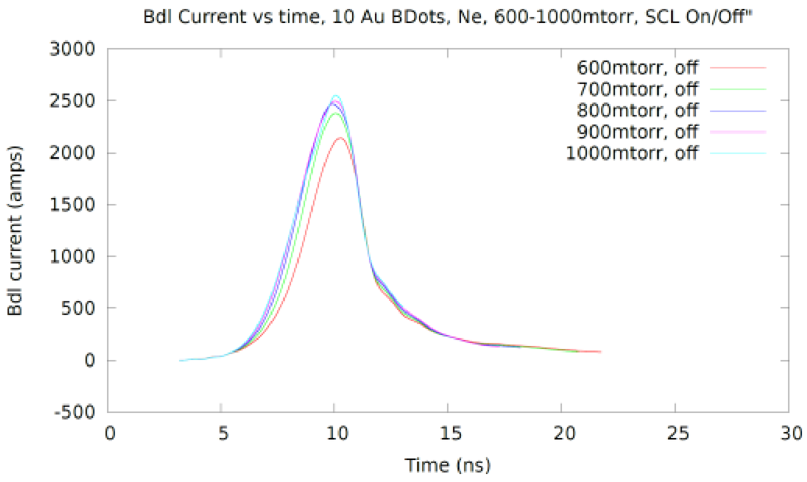


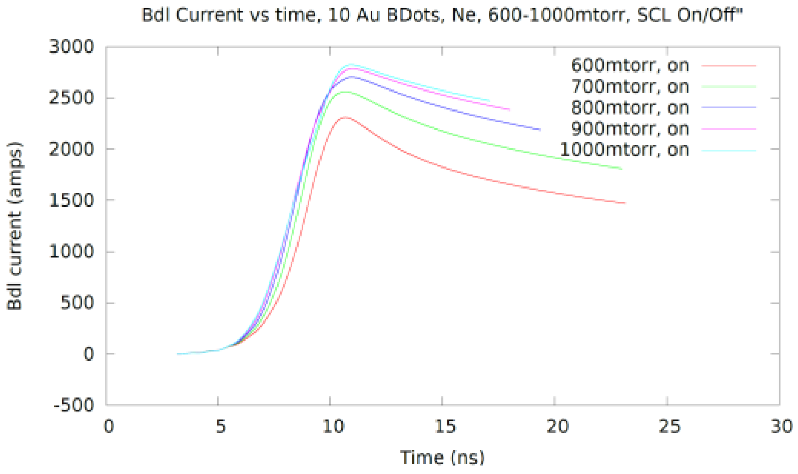
Figure 15a (top): Bdl current vs time for Ne and N_2 B-Dot simulations above 200 mTorr

Figure 15b (bottom): Bdl current vs time comparing Ne and N_2 B-Dot simulations above 200 mTorr

High Pressure Ne SCL Emission Comparison

- Bdl current increases as pressure increases
- However, the rate of increase decreases with each pressure
- This is due to the pressure approaching Ne's minimum in the Paschen curve
- We also see very different tails for the SCL on and off cases





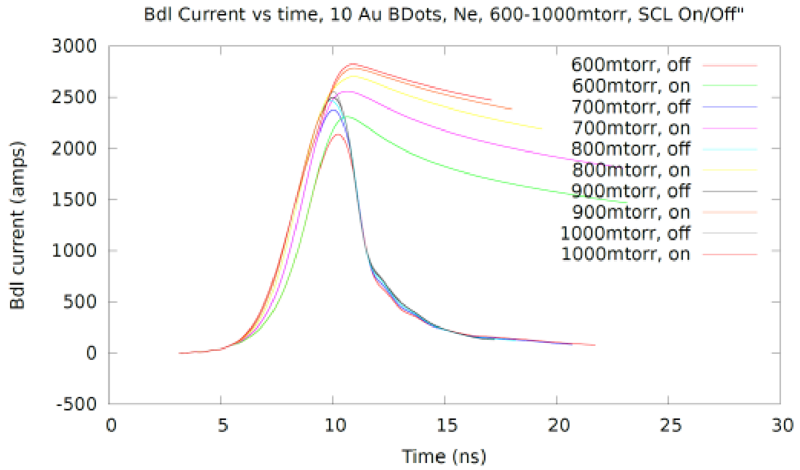
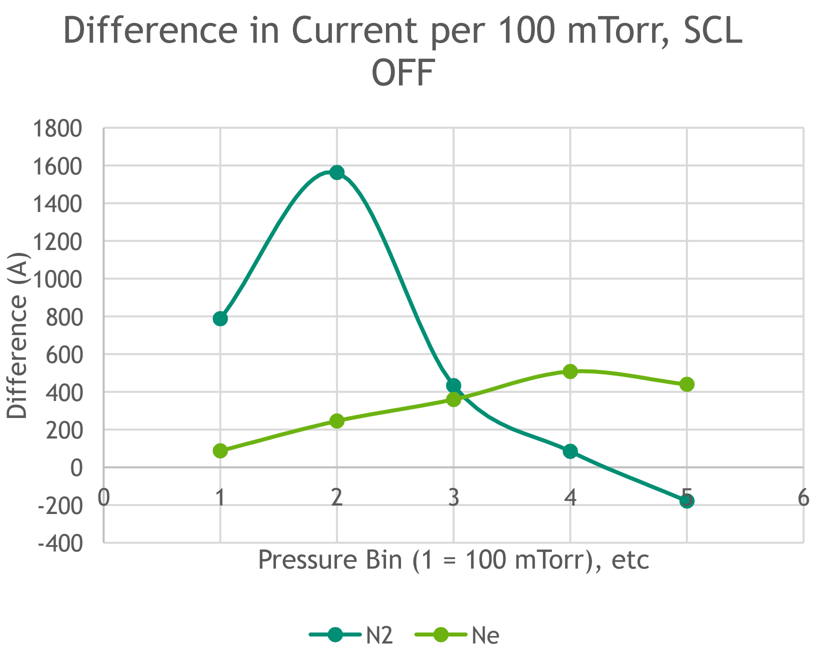
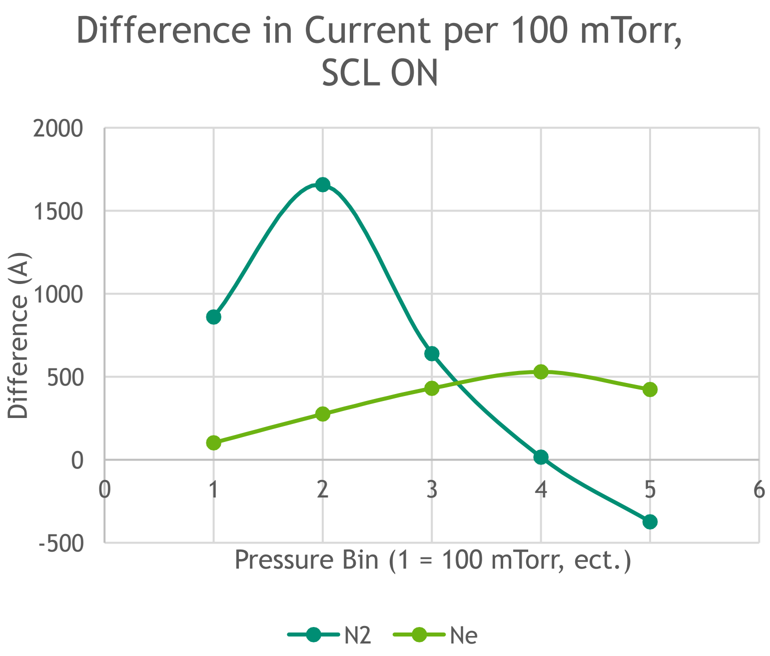


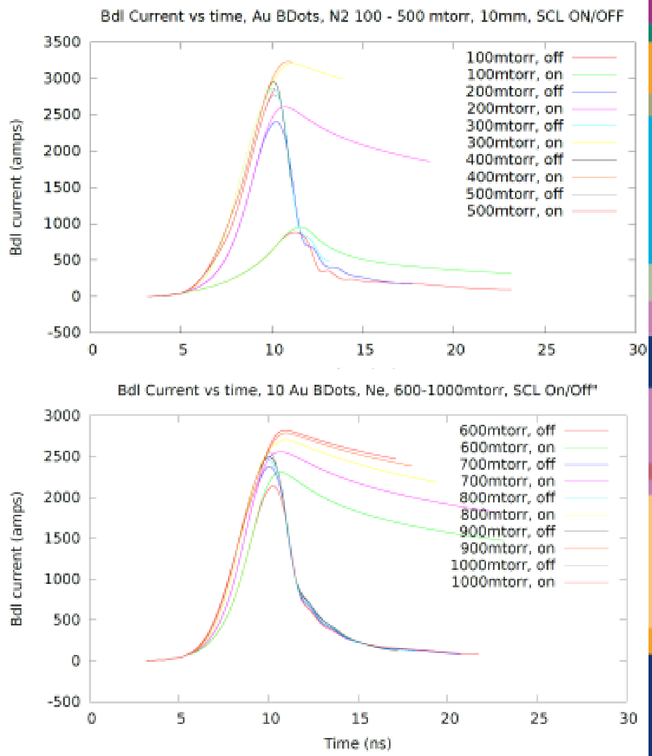
Figure 19a (top): Bdl current vs time for Ne B-Dot simulations above 600 mTorr, SCL on/off

Figure 19b (bottom): Bdl current vs time comparing SCL emission effects for Ne B-Dot simulations above 600 mTorr

Electric Discharge and Bdl Currents







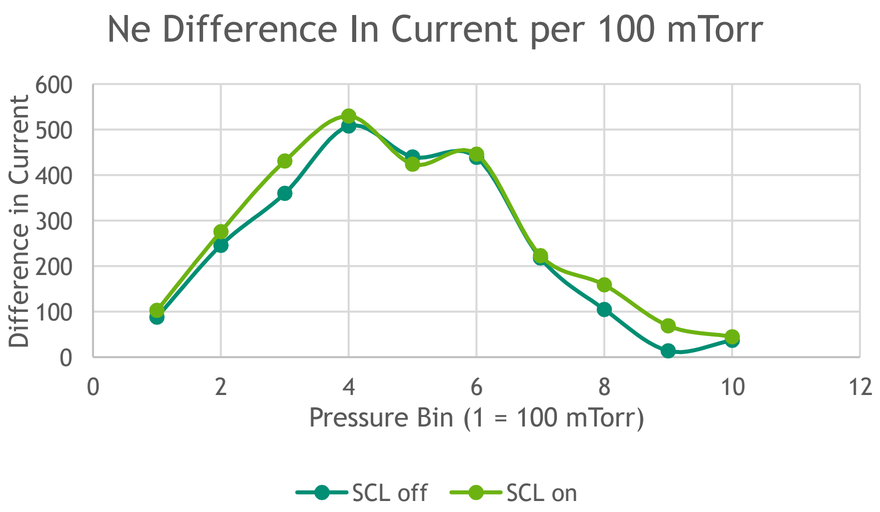


Figure 20. Difference in Bdl current between 100 mTorr pressure bins. The top graphs compare N_2 and Ne, and the bottom graph is Ne for pressures ranging from vacuum to 1torr

Unanswered Questions

1. Of the simulation models (both SCL on/off), which is the real tail of the experiment?
2. Why does the pulse of the SCL off cases oscillate?
3. Where do the double peaks come from in SCL off cases?
4. What does the shape of the pulse from experiment?
    1. The simulated pulses match the experimental data in shape and in time
    2. However, the peak currents in experiment are much higher than in simulation

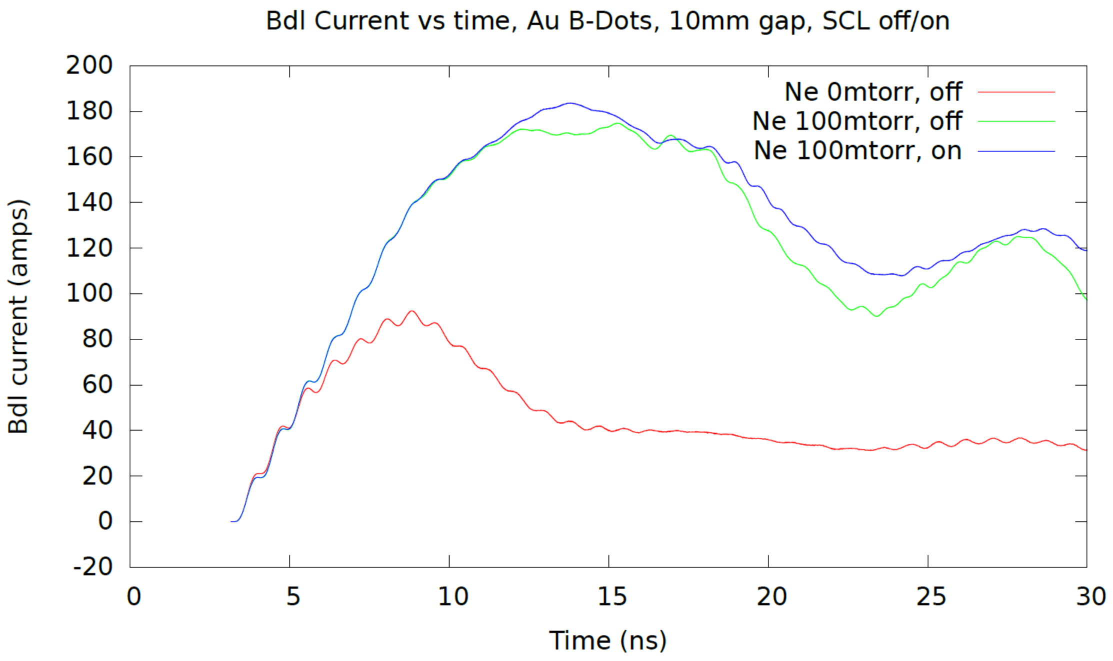


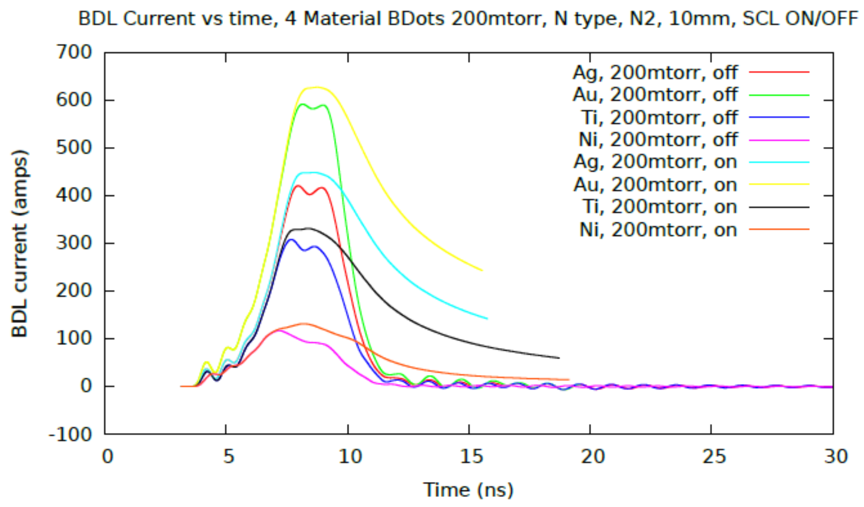
Figure 21: Bdl current vs time for Ne B-Dot simulations below 200 mTorr, SCL on/off, oscillatory

SCL Emission

- Of the simulation models both SCL on/off, which is the real tail of the pulse from experiment?
  - **SCL Emission "on" is simulating the maximum possible current contribution from the surface, SCL "off" is simulating the minimum, or the photoelectron emission only. The tail is somewhere in between "on" and "off"**
- Why does the pulse of the SCL off cases oscillate?
  - **The cavity ringing has the shape of a damped RLC circuit**
  - **The SCL "on" case has less oscillations because it acts like an overdamped RLC circuit**
  - **The pulse can be modeled as an AK gap with plasma physics coupled with a transmission line.**
    - **My master's thesis was demonstrating that coupling a transmission line to an AK gap produces similar physics – this simulation configuration allows greater computational efficiency.**

Double Peaks in Ne and N_2

- As the pressure increases from vacuum, these double peaks are more pronounced [13]
- We see double peaks because the current generated due to the plasma in the AK gap is slightly delayed compared to the initial photoelectron spectrum
  - As the current contributions from the plasma catches up, we see the second peak, which is not as strong as the initial peak
  - We even see a 2^{nd} peak later in the simulation due to an inductive effect after 24ns. However, for N_2 and higher pressure simulations, running for that long would cause the simulation to time-out
- As pressure increases, the rise time decreases



[13]

Figure 6a (top): Bdl current vs time for N_2 B-Dot simulations between at 200 mTorr with SCL on/off for many cathode materials

B-Dot Cold Test

- Proof of concept for circuit modeling
- 10mm Au B-Dot
- Input is a beam of electrons instead of a spectrum of photo
  - No coupling to the MC photon/electron code
- Perfect conductor boundary on top and bottom surfaces
- Reflecting boundary condition on front and back faces
- Absorbing boundary condition on the transmission line
- Quicker run times for easier debugging
- Proves that Bdl current at the cavity is Bdl current in the B-dot

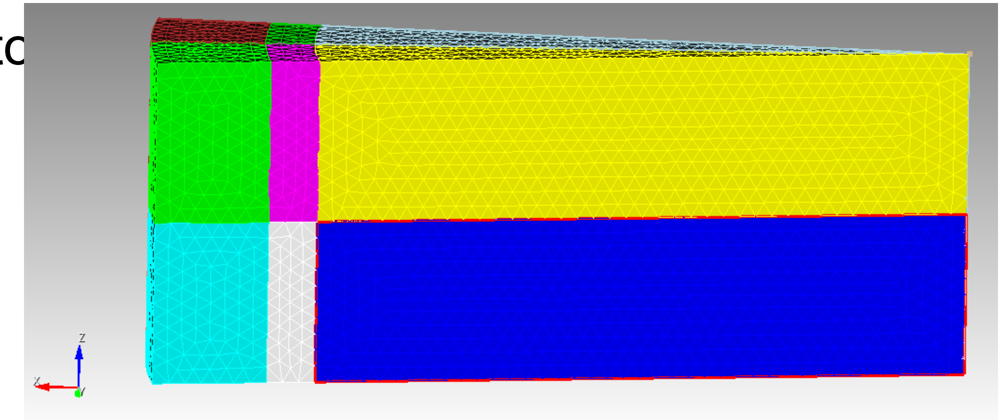


Figure 16: 10mm B-Dot cold test tet-meshed geometry

Circuit Modeling

Final Geometry with diagnostics for B-Dot Cold Test

The blue lines are Edl, Bdl, and Bdl Circle currents

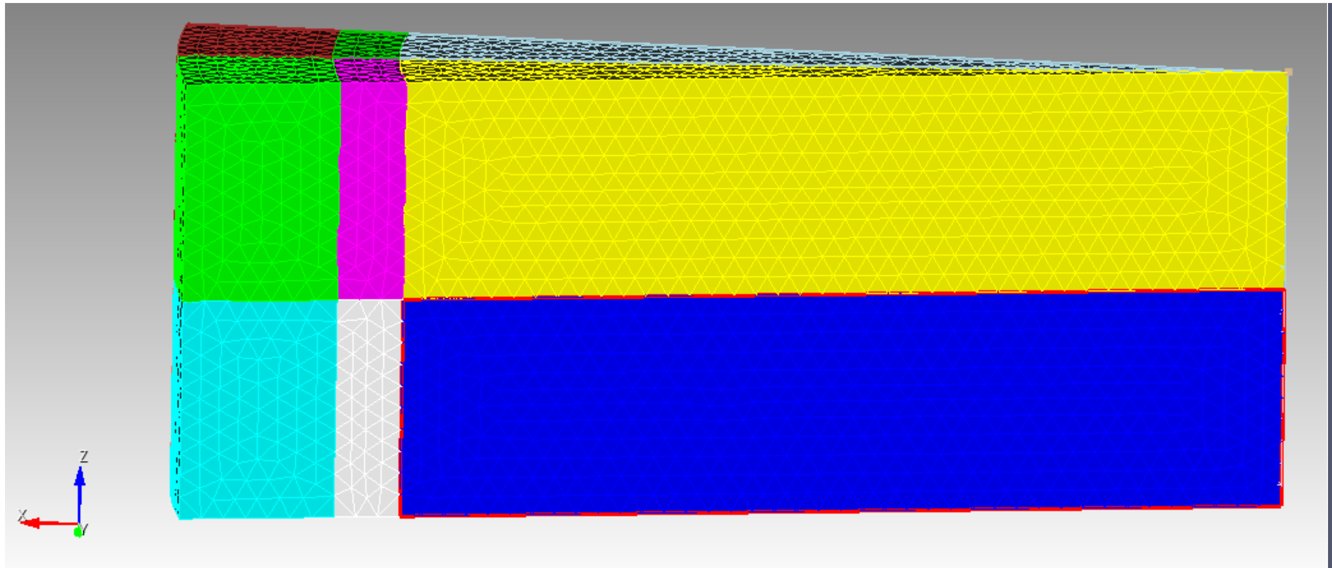


Figure 22: 10mm B-Dot cold test tet-meshed geometry

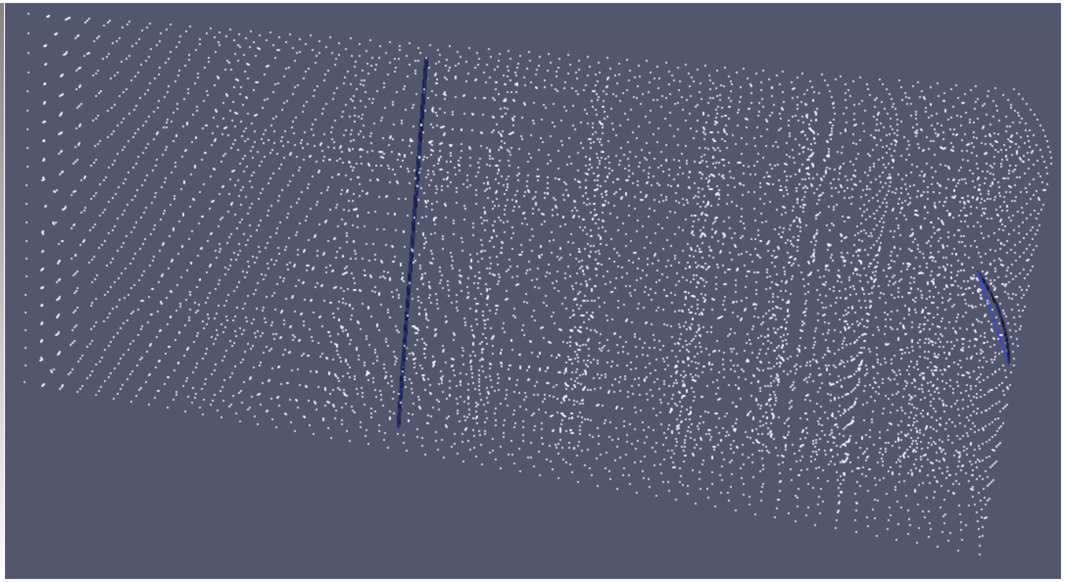


Figure 23: Diagnostics for a 10mm B-Dot cold test geometry. The curved line is Bdl Circle current, the straight horizontal line is Bdl current, and the vertical line is Edl Voltage

Axial TL Diagnostics

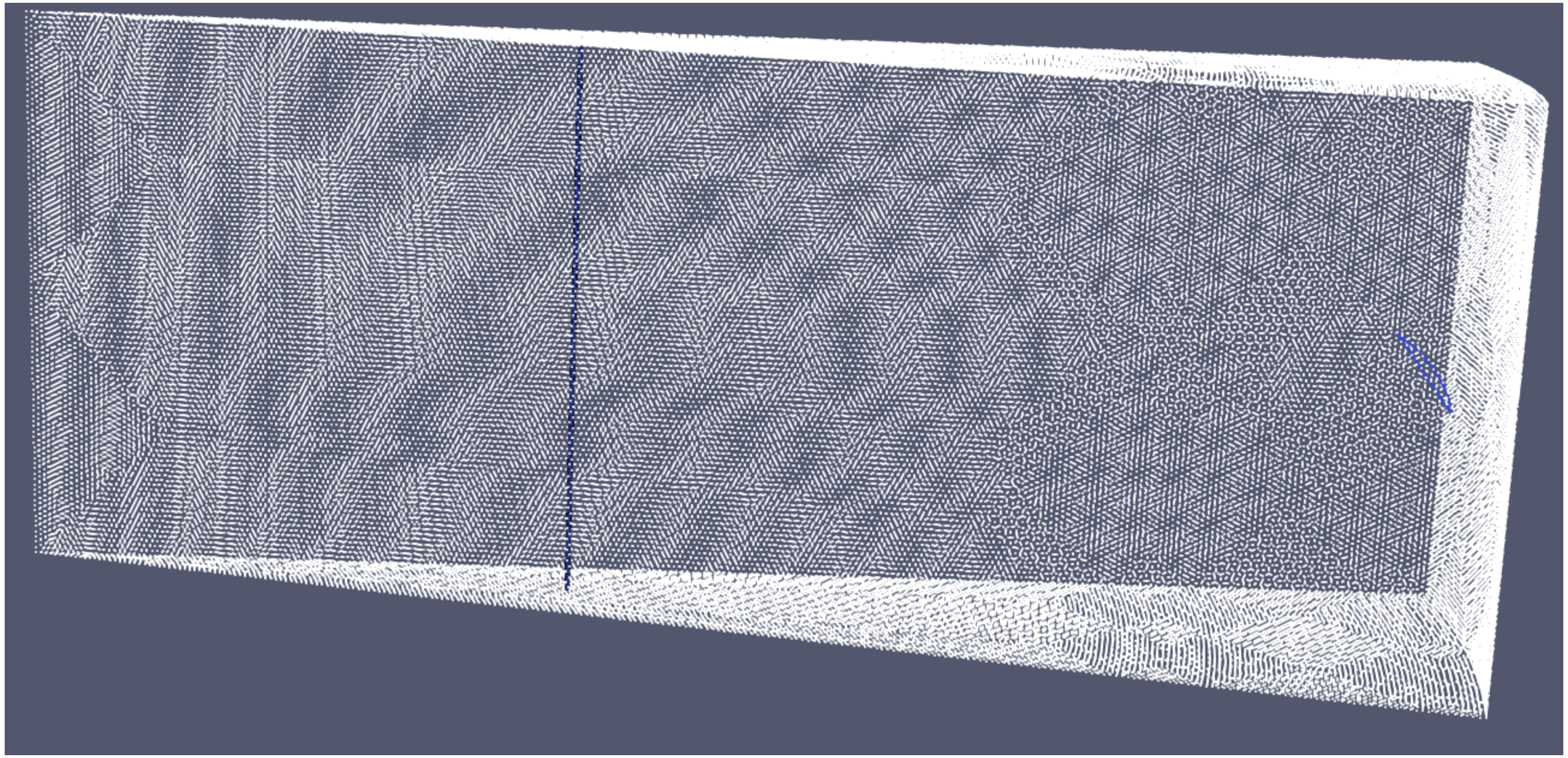


Figure 21: Diagnostics for a finer meshed 10mm B-Dot geometry. The curved line is Bdl Circle current, the straight horizontal line is Bdl current, and the vertical line is Edl Voltage

Axial Transmission Line

Table 2 Capacitance and Inductances for each section along axial transmission line

#Length	num_cells	C_l	L_l	G_l
0.002	20.0	5.910195817843425e-11	1.882594232655415e-07	0.0
0.011	110.0	5.910195817843425e-11	1.882594232655415e-07	0.0
0.01	100.0	6.889189348252632e-12	1.6150667368952925e-06	0.0
0.005	50.0	1.1705623268286148e-10	9.505261108719454e-08	0.0
0.002	20.0	1.1705623268286148e-10	9.505261108719454e-08	0.0

- C_l and L_l are capacitance and inductance per length respectively
  - These were calculated using the formulae in the previous slide
- G_l is conductivity per length
- The lengths (m) are the distances from the TL to the B-Dot cavity in the 3-D simulation
- If L and C are specified from a table, then the side set can be specified without recalculating L and C
- Special mention to Keith and Peggy for this table

Radial Transmission Line Code

```
Circuit Network:
  Transmission Lines:
    TL z:
      Names: [TL z]
      Mode: TEM
      Sideset: surface_3
      Capacitance: {Capacitance}
      Inductance: {Inductance}
      Length: {TL_Z_length} #distance from surface n to the b-dot diagnostic
      Number of Cells: {int(.5 + 10*emission_plate_radius/ref_mesh)}
  Nodes :
    EM Coupling :
      Type : EM Coupling
      Transmission Lines : [TL z]
      Sideset : surface_3
      Conductors : [cathode, anode]
      Ground : anode
```

- TL Z: name of the transmission line
- Surface_3 is the transmission line location on the cavity
- The diagnostics are located at the midpoint of the cavity
- Even though L and C are hardcoded, the simulation will recalculate the values in the “Node” block
    - Although the L and C values are set, the code sees the sideset and computes L and C from there, ignoring my values
    - The node block is essential in specifying the location of the TL

Axial Transmission Line Code

```
Circuit Network:
  Transmission Lines:
    BDot_body:
      Names: [BDot_body]
      Mode: TEM
      Parameters File: TransmissionLine.dat
  Nodes:
    EM Coupling:
      Type: EM Coupling
      Transmission Lines: [BDot_body]
      Sideset: surface_3
      Conductors: [cathode, anode]
      Ground: cathode
    Voltage Source:
      Type: Open Circuit Source
      Transmission Line: BDot_body
      Resistance: 1.0e-12
      Voltage Source Function: |
        Voc = 0;
```

```
  Time History Diagnostics:
# z_bdot = {z_bdot=-mm2m*height/2}
# The wedge now goes from -wedge_angle/2 to wedge_angle/2 instead of 0 to wedge_angle
# rel_angle = {rel_angle=PI*wedge_angle/180.0}
# radius_bdot = {radius_bdot = mm2m*emission_plate_radius*.995}
# radius_edl = {radius_edl=0.5 * aperture_radius * mm2m}
    EDL:
      Line Integral:
        Field: E
        Points: (0.01, 0, {-mm2m*height}), (0.01, 0, 0.0)
        Num Points: {int(10*height/effective_h + 0.5)}
    BDLCurrent:
      Line Integral:
        Field: B
        Multiplier: {current_scale / permeability}
        Points: ({radius_bdot*cos(0.5*rel_angle)}, {radius_bdot*sin(0.5*rel_angle)}, {z_bdot}), ({radius_bdot*cos(-0.5*rel_angle)}, {radius_bdot*sin(-0.5*rel_angle)}, {z_bdot})
        Num Points: {int(10*2*radius_bdot*sin(0.5*rel_angle)/(mm2m*effective_h )+0.5)}
    BDLCurrent_circle:
      Line Integral:
        Field: B
        Multiplier: {current_scale / permeability}
        Circle Center: 0,0, {z_bdot}
        Circle Radius: {radius_bdot}
        Circle Normal: 0, 0, -1
        Num Points: {int(10*2*PI*radius_bdot/(mm2m*effective_h )+0.5)}
```

- Circuit block and the Diagnostics block

1 mm LB-Dot Full Simulation Results

- 1 mm cavity, Ne fill gas, low pressure
- Stainless-Steel input spectrum
- Basis of comparison for transmission line simulations
- LB-Dot: added inductance in the geometry causes higher impedance and more oscillations

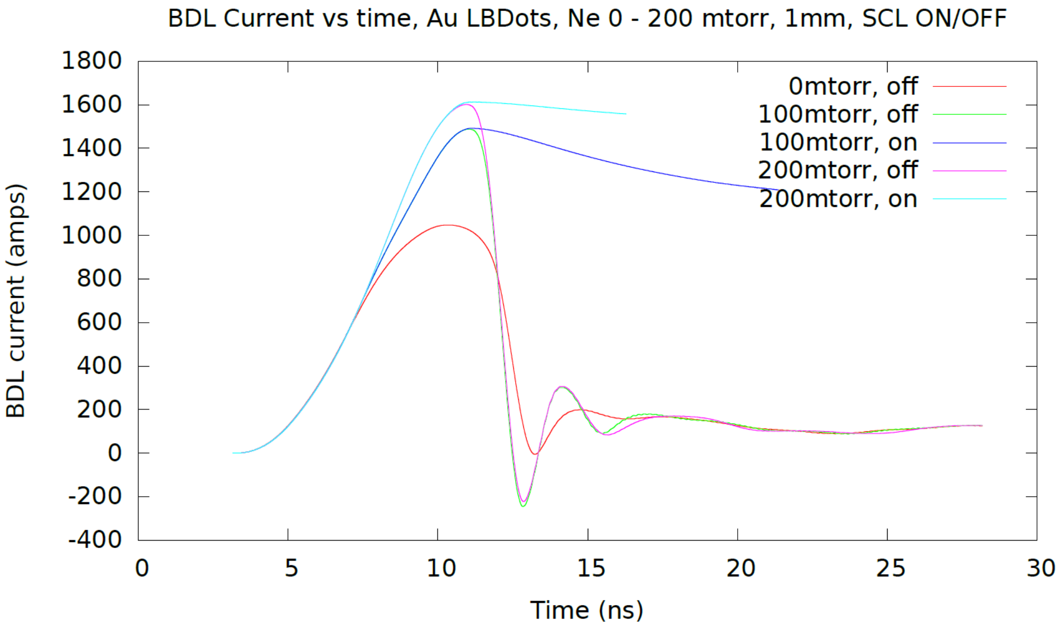
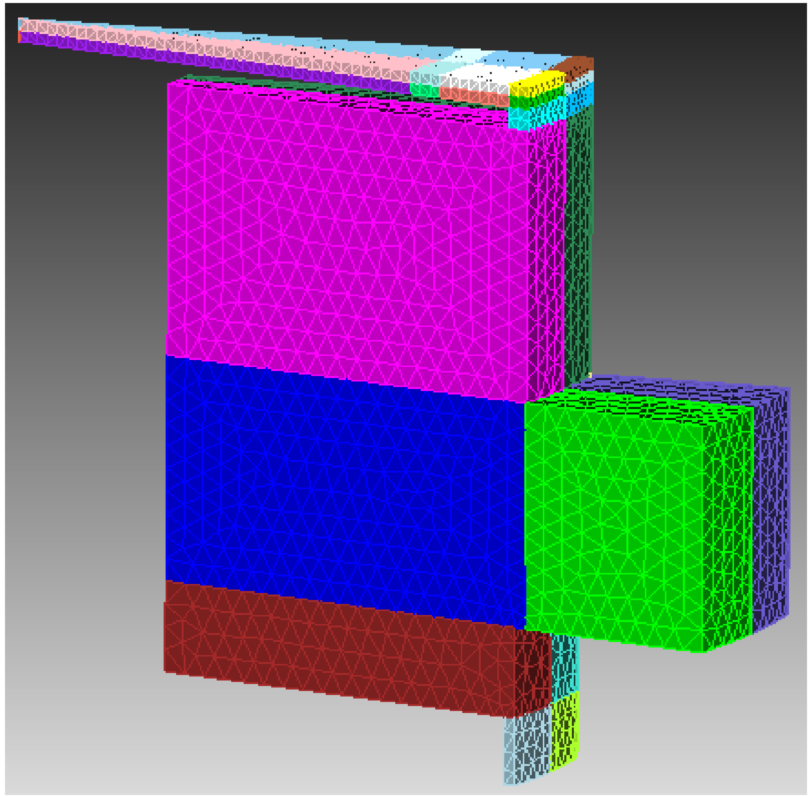


Figure 31: Bdl current vs time for a 1 mm Au LB-Dot system between 0 and 200 mTorr Ne fill gas full simulation results, stainless-steel input spectrum.

Figure 32: 1 mmN LB-Dot full geometry.



1 mm LB-Dot Transmission Line Results

- THIS DIVERGES BADLY, WHY?

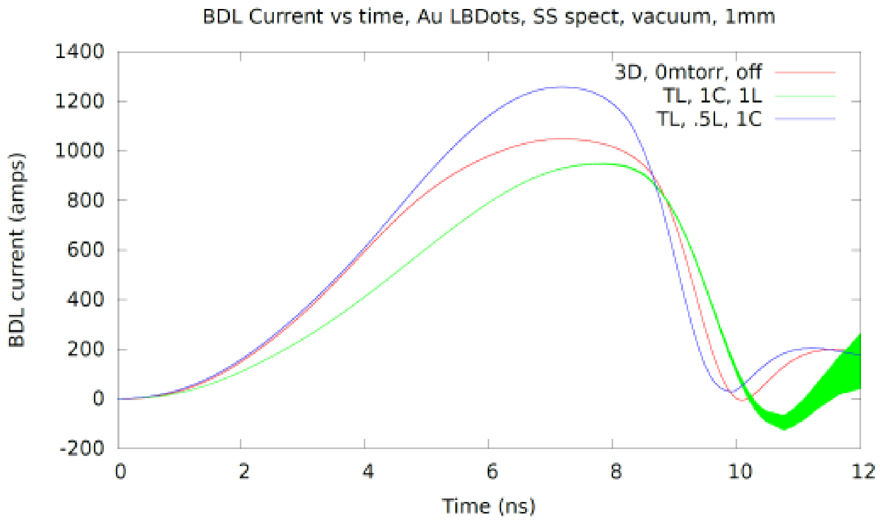
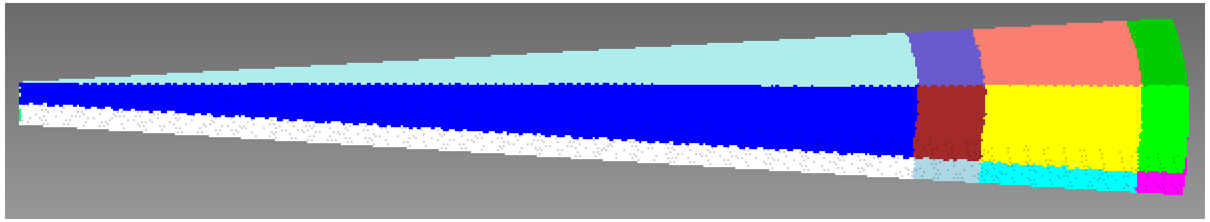


Figure 38: Bdl current vs time for a 1 mmV Au LB-Dot system at vacuum, stainless-steel spectrum, transmission line comparison

1 mm B-Dot Transmission Line Results



- Stainless-steel input spectrum
- High pressure, Ne
- .5L transmission line compared to full simulation (3D)
- Progressively worse as pressure increases
- .5L, 1C

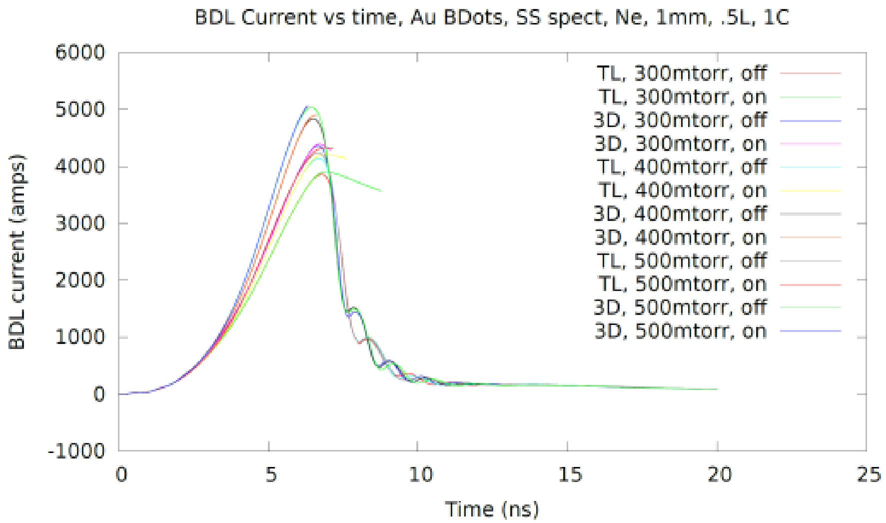
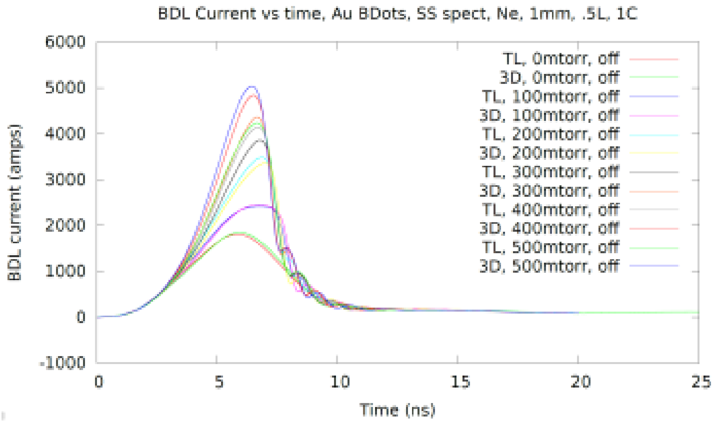
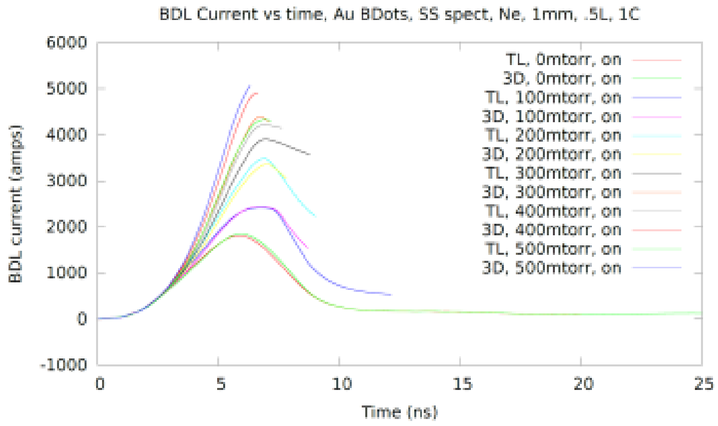


Figure 29a: Bdl current vs time for a 1 mmV Au B-Dot system high pressure Ne (right), stainless-steel spectrum, .5L

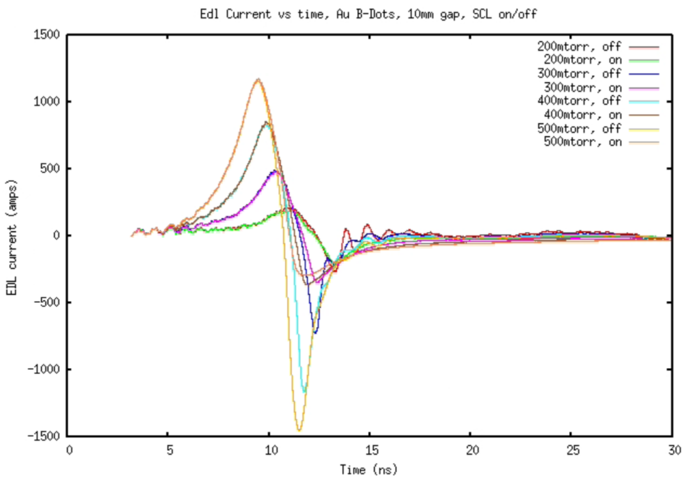
Figure 29b: Bdl current vs time for a 1 mmV Au B-Dot system with Ne fill gas, stainless-steel spectrum, .5L, SCL OFF (left) SCL ON (right)

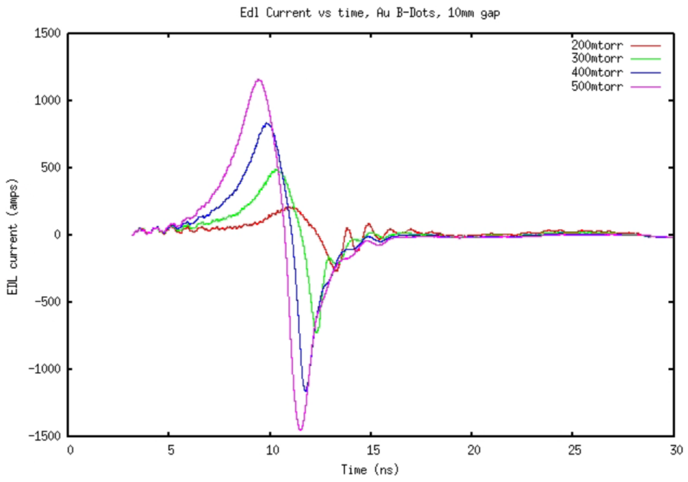


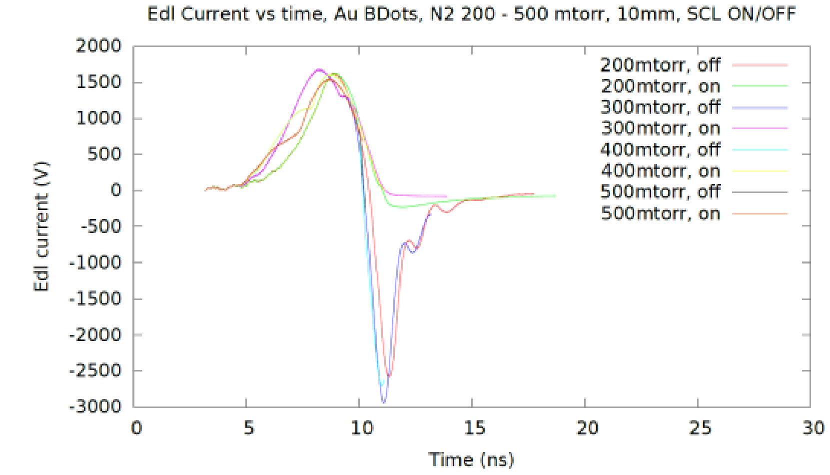


Edl Voltage

- Voltage is the integral of the electric field over length
- SCL emission does not contribute the voltage in the cavity
- We see more oscillations in SCL off cases because it acts as an underdamped LC circuit
- As expected, the voltage in the N_2 fill gas cavity is higher than the Ne fill gas cavity, but it peaks at 300 mTorr

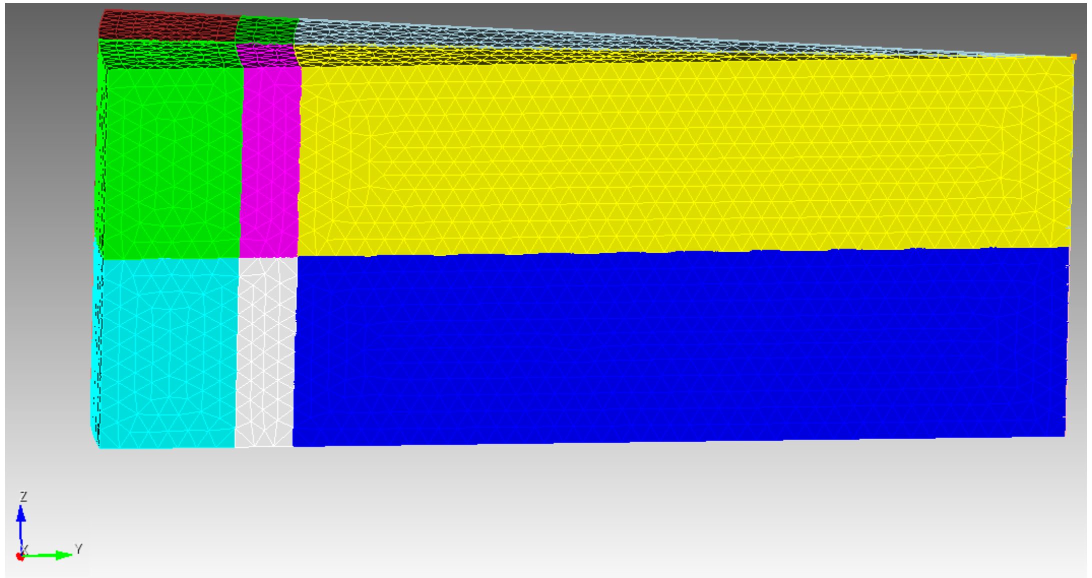






Circuit Modeling

- First attempt
- Notice the orientation with x into the page, and y moving left to right.



Discussion: Coupling MC and EM PIC codes

- "All models are wrong, some are useful".
  - George Box, and many others
- Instead of using a beam of electrons, a photon spectrum to create emitted electrons is more indicative of what will happen in the real world
- Moving between the codes is simple and produces better results
- Modeling the transmission line reduces computation time for similar systems while producing accurate results
  - The only changes are the geometry, initial voltage, irradiation material, and input photon spectrum
- The MC photon/electron code can run in 1D, 2D (cylinder), and 3D
  - Changing the dimension of the code may be able to produce similar results with less computational resources